



CONTRACT NO. A032-170
FINAL REPORT
MARCH 1994

**Development of
Intermedia Transfer Factors
for Toxic Air Pollutants**

***Volume I:
Volatile Organic Compounds***



CALIFORNIA ENVIRONMENTAL PROTECTION AGENCY



**AIR RESOURCES BOARD
Research Division**

Development of Intermedia Transfer Factors for Toxic Air Pollutants

Volume I: Volatile Organic Compounds

Final Report

Contract No. A032-170

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ACKNOWLEDGMENTS

This project was made possible with funding from the California Air Resources Board (Contract No. A032-170) and we are grateful for the helpful discussions and participation of its staff: Ralph Propper (Contract Manager), Janette Brooks, Lynn Terry, Richard Corey, Narcisco Gonzales and Grant Chin. We also thank Robert Clay and Robert van de Water for their assistance. We also appreciate the technical review of the Chromium (VI) report by Dr. Janet Hering. The contribution to the literature database on benzo(a)pyrene from Dr. Douglas Lane (Atmospheric Environment Service, Environment Canada) and his suggestions are also greatly appreciated. We are thankful to Joy Merritt (Senior Editor, Chemical Abstract Service) for detailed discussion of the nomenclature for benzo(a)pyrene. Finally, we express our gratitude to Donato Kusuanco and Jeanne Desilets for their technical assistance in preparing the various components of this report.

This report was submitted in fulfillment of Contract No. A032-170 "Development of Intermedia Transfer Factors for Toxic Air Pollutants" by the University of California, Los Angeles under the sponsorship of the California Air Resources Board. Work was completed as of March 30, 1994.

ABSTRACT

California's regulations for air toxics require the application of multimedia assessment of human health risk. This approach requires knowledge of intermedia transfer factors (ITFs) for specific toxic air pollutants. In order to meet the above need, a critically evaluated information base on ITFs was developed for a selected number of air toxics. The specific chemicals were selected in order to allow the assessment of ITFs for the following chemical classes: (1) volatile organics (benzene); (2) hydrophilic/reactive volatile organic compounds (formaldehyde); (3) volatile chlorinated low molecular weight hydrocarbons (methylene chloride); (4) particle-bound organics (benzo(a)pyrene and 2,3,7,8-TCDD); (5) reactive metals (chromium VI); and (6) metals that are mobilized through formation of organo-metallic compounds (mercury). Experimental data and estimates of ITFs for the above chemicals were critically evaluated. Detailed reports for seven compounds were prepared and are available as separate chemical-specific volumes of ITF information. The complete set of chemical-specific ITF volumes prepared in this project should provide a useful resource for future development of ITF estimation methods for specific chemical classes.

VOLUME I: VOLATILE ORGANIC COMPOUNDS

TABLE OF CONTENTS

Disclaimer	i
Acknowledgments	ii
Abstract	iii
Table of Contents	iv
Executive Summary	v

Section 1. Benzene

Section 2. Methylene Chloride

Section 3. Formaldehyde

EXECUTIVE SUMMARY

Toxic air pollutants which are released to the atmosphere as the result of a variety of human-related activities (air emissions and/or direct discharge to surface water, etc.) move across environmental boundaries and are therefore found in most media (Figure 1.1). Therefore, it is logical to employ a multimedia approach for a comprehensive and integrated approach to evaluating the risks associated with toxic air pollutants.

Indeed California's air pollution regulations for air toxics are deeply rooted in the process of multimedia assessment of human health risk. The assessment of human health risks requires the determination of exposure of the human receptor to pollutants from multiple pathways. The approach requires an understanding of the complex physical, chemical, and biological processes that govern the movement of pollutants through environmental media. For example, in one of the approaches recommended by the State of California Environmental Protection Agency (CALEPA), given monitored or modeled atmospheric concentrations of air toxics, one can resort to appropriate empirical or theoretical algorithms to estimate the transfer, and thus, the accumulation of the pollutants of interest in both non-biological media (e.g., atmosphere, surface water, soil) and biological media (e.g., fish, cattle, vegetation). The resultant media concentrations can then be used to estimate the total dose (or average daily dose) of the given air toxic contaminants and subsequently the associated human health risks (Figure 1.2). The above multipathway exposure analysis involves a variety of chemical-specific intermedia transfer factors (ITFs). These ITFs are needed to estimate the rate of movement of chemicals from one medium to another as well as their level of accumulation in various environmental compartments (e.g., water, soil, vegetation).

Although the multimedia approach to exposure analysis and risk assessment is attractive, its implementation is often accompanied with uncertainties. These uncertainties arise from the lack of data in some areas (e.g., dose-response data, population activity patterns, environmental chemical concentrations), which leads to reliance on models where certain assumptions and default parameter values are introduced. Generally, the

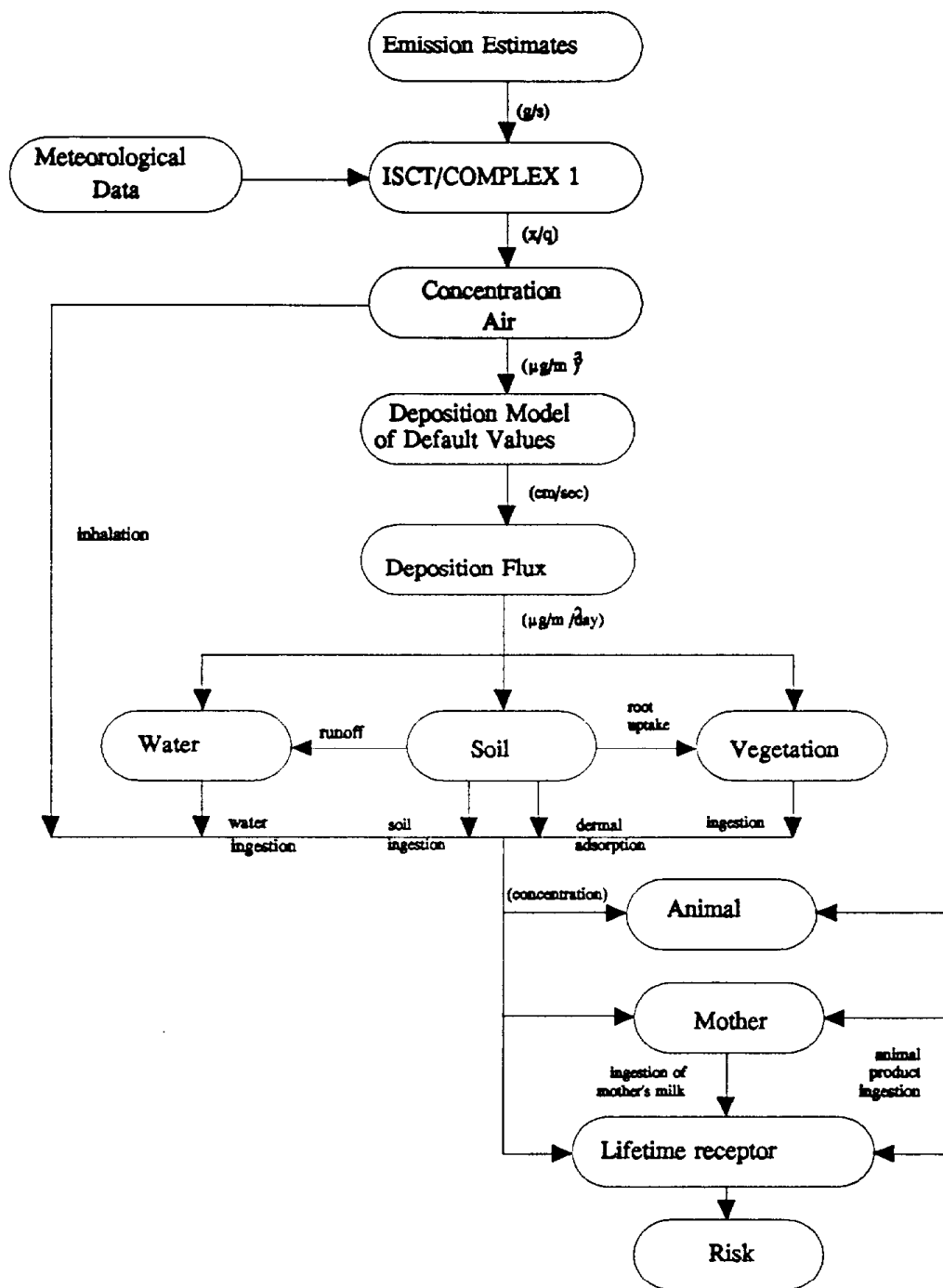


Figure 1.1 Exposure Flowchart

(Source: "Health Risk Assessment Guidelines for Non-Hazardous Incinerators", ARB/DHS, August 1990)

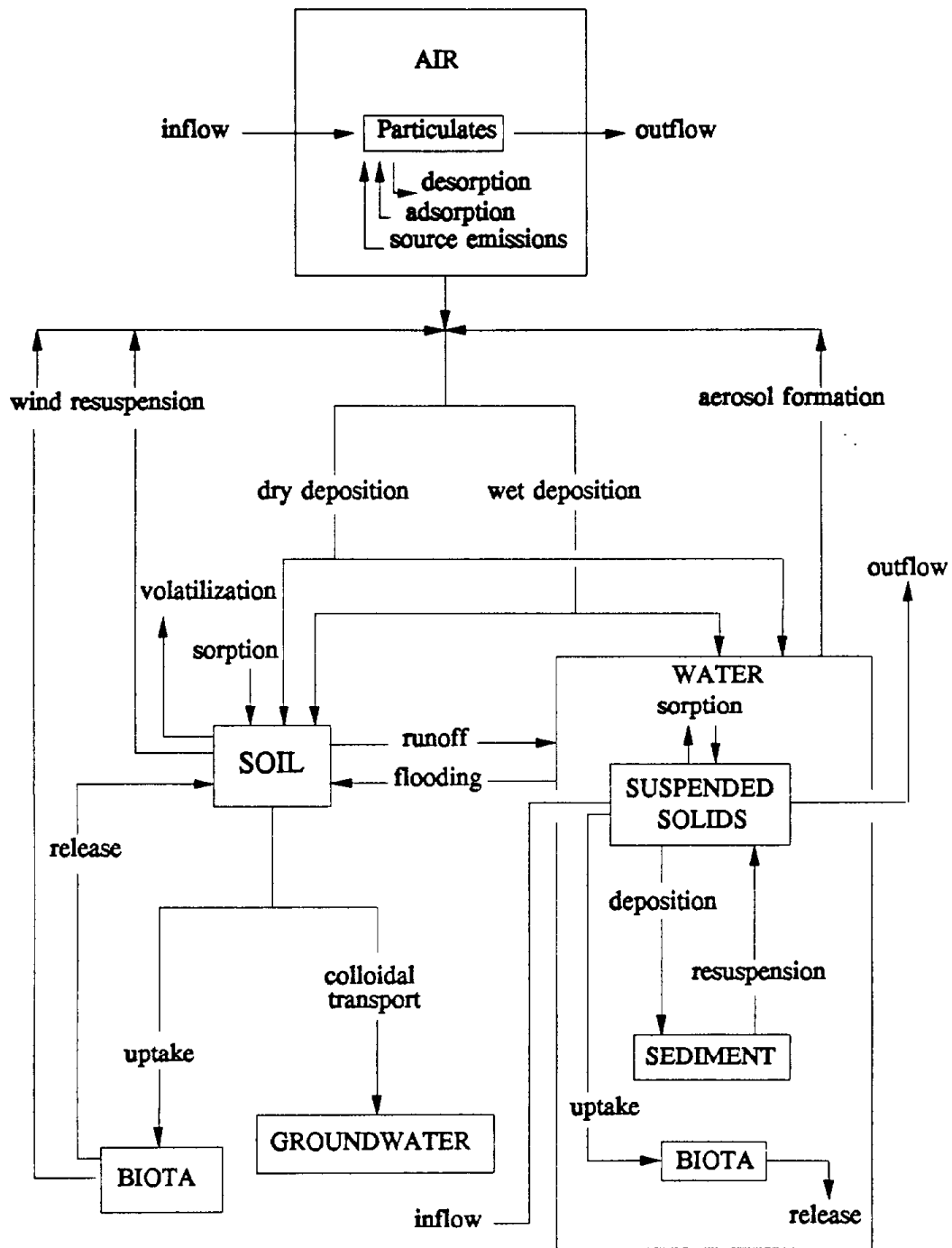


Figure 1.2 Schematic of Multimedia Transport Processes of Particle-Bound Pollutants

assumptions employed and the use of default parameter values are designed to err on the side of human health protection to avoid underestimating risk to the public. Major sources of uncertainty which may either overestimate or underestimate risk for toxic air pollutants include:

- Extrapolation of toxicity data in animals to humans;
- Air dispersion modeling;
- Estimation of emissions; and
- Analysis of multimedia exposure.

This study focused on the last category of multimedia exposure analysis which requires knowledge of intermedia transport processes. Uncertainties in the predictions of multimedia exposure analysis is the consequence of both the lack of understanding of some intermedia transport processes and the frequent use of approximate treatments of intermedia transport processes and estimated intermedia transport factors. Such uncertainties can be reduced by using the most accurately available intermedia transfer factors such as pollutant physicochemical, partitioning, mass transfer and degradation parameters.

This study provides information on some of the major intermedia transfer factors (ITFs) used in a number of different multimedia models including the CAPCOA (1992) guidelines. These guidelines provide procedures for preparation of health risk assessments required under AB 2588. Under some circumstances, the CAPCOA (1992) guidelines allow for submission of an uncertainty analysis associated with the risk assessment. Thus, chemical-specific ITF information should be valuable for assessing uncertainty analyses submitted to the California Air Resources Board (CARB).

In order to meet the above needs, a critically evaluated information base on ITFs was developed for a selected number of air toxics. The specific chemicals were selected in order to allow the assessment of ITFs for the following chemical classes: (1) volatile organics (benzene); (2) hydrophilic/reactive volatile organic compounds (formaldehyde); (3) volatile chlorinated low molecular weight hydrocarbons (methylene chloride); (4) particle-bound

organics (benzo(a)pyrene and 2,3,7,8-TCDD); (5) reactive metals (chromium VI); and (6) metals that are mobilized through formation of organo-metallic compounds (e.g., mercury). Experimental data and estimates of ITFs were critically evaluated and detailed specific reports were prepared and are part of this final report. The complete set of ITF reports (see Table 1) prepared in this project should provide a useful resource for future development of ITF estimation methods for specific chemical classes.

The overall objective of the individual ITF reports is to present information on chemical-specific intermedia transfer factors which is pertinent for multimedia exposure pathways estimation and for health risk assessments. The purpose of the chemical-specific ITF reports is to: (1) critically review existing literature to determine pertinent intermedia transfer parameters for the study chemicals; (2) evaluate and update intermedia transfer factors currently used in multimedia exposure estimations; and (3) provide pollutant-specific estimates where no data are available or where default values are used.

Since the results of this study may be used to support efforts in multipathway analysis of exposure to the study chemicals, a number of multimedia contaminant transport models were reviewed in terms of algorithms, default values, underlying assumptions, and the influence of the overall logic on the estimates of risk. Based on this review, selected physicochemical properties, partition coefficients, and intermedia transport coefficients were critically evaluated.

TABLE 1

**INTERMEDIA TRANSFER FACTORS FOR
MULTIPATHWAY EXPOSURE ANALYSIS:
COMPOUND CLASSES AND CHEMICALS STUDIED**

Chemical Class	Specific Chemical Reviewed	Volume Number
Volatile Organics Hydrocarbons	Benzene	I
Reactive Metals	Chromium VI	II
Particle-Bound Organics	2,3,7,8-TCDD	III
Volatile Chlorinated Low Molecular Weight Hydrocarbons	Methylene Chloride	IV
Particle-Bound Organics (PAH Group)	Benzo(a)pyrene	V
Metals Mobilized through Formation of Organo- Metallic Compounds	Mercury	VI
Hydrophilic/Reactive Volatile Organic Compounds	Formaldehyde	VII

Physicochemical Properties

Physicochemical properties are important for the analysis of intermedia transport parameters such as mass transfer coefficients and for the determination of parameters such as partition coefficients, biotransfer factors, and mass transfer coefficients. The specific physicochemical parameters considered in this study are given below.

- Water Solubility;
- Vapor Pressure;
- Density;
- Molar Volume;
- Boiling Point;
- Molecular Weight;
- Melting Point; and
- Heat of Vaporization.

Partition Coefficients

Once released to the environment, toxic air pollutants will be distributed to various compartments due to various transport processes. The net chemical transport from one compartment to another may be limited by equilibrium constraints which are quantified by appropriate partition coefficients. The partition coefficient, H_{ij} is generally defined as

$$H_{ij} = C_i/C_j$$

where C_i and C_j are the concentration in compartment i and j , respectively, at equilibrium. In this study, the following partition coefficients were considered:

- Henry's Law Constant;
- Octanol-Water Partition Coefficient;
- Gas Phase/Particle Partitioning Coefficient;
- Soil/Water-Organic Carbon Partition Coefficient;
- Bioaccumulation Factors; and
- Bioconcentration Factors.

It is noted that bioaccumulation factors and bioconcentration factors often represent steady-state concentrations rather than an equilibrium state. These factors are also at times based on the total chemical concentration which includes particle-bound and dissolved forms of the chemical under consideration; thus, in such cases, the reported bioconcentration factors do not represent thermodynamic constraints and simply represent the partitioning obtained for the particular set of experimental conditions for which these factors were obtained.

Transport Parameters

The transport of toxic air pollutants in the environment is governed by either convective transport in a given medium (not addressed in this report) or intermedia transport from one environmental compartment to another. It is important to note that some chemicals (e.g., semi-volatile organics) can be present in both the gaseous and particle-bound forms. Thus, the exchange of such chemicals between the atmosphere and the terrestrial and aquatic environments depends on both the dry and wet deposition of their gaseous and particle-bound forms, as well as on wind resuspension. The relevant intermedia transfer and transformation parameters considered in this study include:

- Diffusion Coefficients in Air and Water;
- Mass Transfer Coefficients for Air/Water Exchange;
- Dry Deposition Velocity;
- Precipitation Scavenging;
- Colloidal Transport in Soils and Sediment/Water;
- Biotransfer Factors; and
- Chemical and Biotransformations.

These intermedia transport parameters are defined and discussed in detail in each of the chemical-specific ITF reports. In addition, a brief discussion is provided of the available information on bioavailability and the implication for its accumulation in biological receptors. Finally, the chemical and biotransformations of the study chemicals in each of the major environmental media (i.e., air, water, soil and sediment) are reviewed and the range of relevant reaction half-lives are summarized and discussed.

The evaluation of the above ITFs was carried out for seven chemicals (see Table 1) that are relevant for the determination of the behavior of the study chemicals in various media and the food chain after their release into the atmosphere from stationary and mobile sources. Reported values for the selected parameters were compiled and evaluated. In cases where a wide range of values were reported from different studies, the reported experimental and estimated ITFs were reviewed to assess the reliability of the reported parameter values. Data in the ITF tables are arranged by decreasing order of reliability. Measured values of known uncertainty are considered the most reliable and are thus listed first. Measured values reported without estimates of uncertainty are listed next, followed by calculated values reported with the corresponding prediction equations and reported uncertainty estimates. Calculated values reported without their associated estimation equations were reported last.

Each one of the chemical-specific ITF reports (see Table 1) is a self-contained volume that provides an overview of the nature of the chemical considered, its entry route to the environment, environmental chemical and bio-transformations, definitions of the various intermedia transfer factors considered in the study, a critical evaluation of ITF data and estimation methods, a summary of recommended ranges of ITF values, chemical-specific ITF estimation methods, and recommendations for future improvements in estimating ITFs for the study chemicals.

Development of Intermedia Transfer Factors for Toxic Air Pollutants

Volume I: Volatile Organic Compounds *Section 1 - Benzene*

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ABSTRACT

An information base was developed on the physicochemical and transport parameters for benzene which can be used for the purpose of multipathway exposure assessment. The environmental literature was critically reviewed to: (1) determine the intermedia transfer factors relevant to benzene; (2) evaluate measured values; and (3) recommend estimation techniques applicable to benzene (and homologous compounds) for use in the absence of measured values.

TABLE OF CONTENTS

ABSTRACT	i
TABLE OF CONTENTS	ii
LIST OF FIGURES	iv
LIST OF TABLES	v
1.0 INTRODUCTION AND BACKGROUND	1
2.0 OBJECTIVES	2
3.0 METHODOLOGY	2
3.1 Literature Review	6
3.2 Selection of Parameters	6
3.2.1 Physicochemical Parameters	6
3.2.2 Partition Coefficients	7
3.2.3 Intermedia Transport Parameters	8
3.2.4 Degradation Processes	8
4.0 PRESENTATION OF RESULTS	10
4.1 Physicochemical Parameters	11
4.1.1 Solubility of Benzene in Water	11
4.1.2 Vapor Pressure of Benzene as Cited in the Environmental Literature	12
4.1.3 Molar Volume of Benzene	17
4.1.4 Boiling Point Temperature of Benzene	20
4.1.5 Molecular Weight of Benzene	23
4.2 Partition Coefficients	23
4.2.1 Henry's Law Constant for Benzene	23
4.2.2 Octanol-Water Partition Coefficient for Benzene	24
4.2.3 Soil/Water-Organic Carbon Coefficient for Benzene	27
4.2.4 Bioconcentration Factors for Benzene	30
4.2.5 Biotransfer Factors for Benzene in Milk, Beef, and Eggs	40
4.2.6 Bioconcentration in Beef	45
4.2.7 Bioavailability and Pharmacokinetics of Benzene	45
4.3 Intermedia Transport Parameters	47
4.3.1 Diffusion Coefficients of Benzene in Air and Water	47
4.3.2 Gaseous Mass Transfer Across the Air-Water Interface	51
4.3.2.1 Air/Water - Air Side - Mass Transfer Coefficient (k_g) for Benzene	53
4.3.2.2 Air/Water - Liquid Side - Mass Transfer Coefficient (k_l) for Benzene	58

4.3.3	Dry Deposition Velocity for Benzene	63
4.3.4	Wet Deposition	68
4.4	Degradation	69
4.4.1	Reaction Half-life of Benzene in Air	69
4.4.2	Biodegradation of Benzene in Water and Soil	73
5.0	CONCLUSIONS AND RECOMMENDATIONS	79
6.0	REFERENCES	82

LIST OF FIGURES

Figure 4.1	Gas-Side Mass Transfer Coefficient for Benzene at 20° C for Water/Air Mass Transfer at Large Fetch. (Based on the Correlation of Brutsaert, 1975).	57
Figure 4.2	Liquid-Side Mass Transfer Coefficient for Benzene for Water/Air Mass Transfer at Large Fetch. (Based on the Theoretical Correlation of Cohen and Ryan, 1985).	59
Figure 4.3	Liquid-Side Mass Transfer Coefficient for Benzene at 20° C for a Flowing River.	61
Figure 4.4	Overall Liquid-Side Mass Transfer Coefficient for Benzene for Water/Air Mass Transfer at Large Fetch. (Based on the Theoretical Correlations of Cohen and Ryan, 1985 and Brutsaert, 1975).	64

LIST OF TABLES

Table 1-1	Summary of Representative Values or Estimation Equations for Required Input Parameters for Multimedia Assessment of Benzene . . .	3
Table 4-1	Solubility (S) of Benzene in Water	13
Table 4-2	Vapor Pressure (P_{vp}) of Benzene as Cited in the Environmental Literature	18
Table 4-3	Molar (V_b) Volume of Benzene	21
Table 4-4	Examples of Boiling Point (T_{BP}) Reported in the Literature for Benzene	22
Table 4-5	Henry's Law Constant (H) for Benzene	25
Table 4-6	Octanol-Water Partition Coefficient (K_{ow}) for Benzene	28
Table 4-7	Soil/Water-Organic Carbon Coefficient (K_{oc}) for Benzene	31
Table 4-8	Bioconcentration Factor (BCF) for Benzene in Aquatic Organisms	33
Table 4-9	Root Uptake and Air-to-Leaf Bioconcentration Factors for Benzene .	38
Table 4-10	Feed to Milk Transfer Factor (B_m) for Benzene	43
Table 4-11	Feed to Meat Transfer Factor (B_b) for Benzene	46
Table 4-12	Diffusion Coefficient (D) in Air and Water for Benzene	49
Table 4-13	Dry Deposition Velocity (V_d) for Benzene	65
Table 4-14	Reaction Half-life ($\tau_{1/2}$) of Benzene in Air	71
Table 4-15	Biodegradation Rate Constants/Half-lives ($\tau_{1/2}$) for Benzene	74

1.0 INTRODUCTION AND BACKGROUND

The assessment of health risk requires the determination of exposure of the human receptor to pollutants from multiple pathways. The movement of chemicals throughout the environment is particularly important to the overall assessment of the exposure to toxic air pollutants since airborne pollutants can be deposited to the soil and water, and can be accumulated in plants and animals. Determination of the concentrations of toxic air pollutants in the various environmental media can be obtained by either pollutant transport modeling or field measurements. Both approaches require an understanding of the complex physical, chemical, and biological processes that govern the movement of pollutants through environmental media. In particular, knowledge of the intermedia transfer factors that govern the multimedia partitioning of chemicals in the environment is required for multipathway exposure and risk assessment.

There are, however, uncertainties in the process of multimedia risk assessment. The uncertainties arise from the lack of data in various areas leading to reliance on assumptions and default parameters. Generally, the assumptions employed and default parameters are designed to err on the side of human health protection to avoid underestimating risk to the public (e.g., CAPCOA Guidelines, 1992). Major sources of uncertainty which can affect the estimation of human health risk include:

- Extrapolation of toxicity data in animals to humans;
- Air dispersion modeling;
- Estimation of emissions; and
- Analysis of multimedia exposure.

In this report, the final major source of uncertainty listed above, analysis of multimedia exposure, is addressed. By identifying the input parameters most critical to multimedia analysis and reviewing the reported values and estimation techniques, this report should help characterize and minimize the uncertainty associated with estimating risk from multimedia exposure to benzene. A summary of representative values and estimation

methods for intermedia transfer factors for benzene is given in Table 1-1. Although the presented values only apply to specific conditions, these parameter values have been included for comparison purposes. Finally, the parameter values and estimation methods are discussed in Sections 2 - 5.

2.0 OBJECTIVES

The overall objective of this report is to present information on intermedia transfer factors (ITFs) that is pertinent to the prediction of the transfer of benzene between media such as air, water, soil, and biota in order to refine the multipathway exposure component of health risk assessments. The intermedia transfer factors for benzene presented in this report were obtained based on: (1) review of the pertinent literature; (2) evaluation of intermedia transfer factors currently used in multipathway exposure assessments; and (3) pollutant-specific estimates of ITFs where default values are now used, or no value is available.

3.0 METHODOLOGY

In this study, a thorough investigation was made of the literature values reported for key factors and parameters which govern the partitioning of benzene in the various important compartments and the food chain, following benzene's release to the atmosphere from stationary and mobile sources. Whenever possible, the reported values for a given parameter were placed on a common basis of units and conditions, and the parameter values were critically evaluated. Where no reliable parameter values are found in the literature or default values are currently being used in the CAPCOA multipathway exposure analysis, pollutant-specific estimates are provided. The details of the methods used, and the parameters investigated, are discussed below.

**Table 1-1. Summary of Representative Values or Estimation Equations for Required
Input Parameters for Multimedia Assessment of Benzene**

Input Parameter	Representative Measured (or Calculated) Values	Units^(a)	Temperature (K)	Estimation Equation	Source Cited	Corresponding Section in Text
S	0.0228 ± 0.0006	mol/L	298	(a)	McAuliffe, 1966	4.1.1
P _{vp}	12.7	kPa	298	(a)	Zwolinski and Wilhoit, 1971	4.1.2
V _b	0.0965	L/mol	(b)	(a)	Lee, 1975	4.1.3
T _{BP}	(353)	K	NA	T = B/(A - log ₁₀ P) - C	Lyman et al., 1990	4.1.4
MW	78.114	g/mol	NA	(a)	IUPAC	4.1.5
H	0.555 ± 0.033	kPa m ³ /mol	298	(a)	Mackay et al., 1979	4.2.1
log K _{ow}	2.13 ± 0.01	dimensionless	298	(a)	Fujita et al., 1964	4.2.2
K _{oc}	31-1023 ^(c)	dimensionless	NR	(a)	See Section 4.2.3	4.2.3
BCF	(9 ± 2 orders of magnitude in the 95% confidence limit)	dimensionless	NR	log BCF = 2.791-0.594 (log S)	Kenaga and Goring, 1978	4.2.4
B _{vd}	(1.9 - 17) ^(d)	dimensionless	281-298	log B _{vd} = 1.588-0.5781 log K _{ow}	Travis and Arms, 1988	4.2.4
B _{vw}	NA	dimensionless	NR	B _{vw} = (0.82 + 0.028 K _{ow} ^{0.77})/K _d	Briggs et al., 1982	4.2.4
B _{ww}	(0.12 - 34)	dimensionless	NR	Eqs. 4-19 to 4-23	See Section 4.2.4	4.2.4
B _m	(3.4 × 10 ⁻⁵) ^(e)	d/kg	NR	B _m = -8.10 + log K _{ow}	Hattemer-Frey and Travis, 1990	4.2.5
B _b	(1.1 × 10 ⁻⁶) ^(e)	d/kg	NR	B _b = -7.735 + 1.033 log K _{ow}	Hattemer-Frey and Travis, 1990	4.2.5

**Table 1-1. Summary of Representative Values or Estimation Equations for Required
Input Parameters for Multimedia Assessment of Benzene**
(Continued)

Input Parameter	Representative Measured (or Calculated) Values	Units	Temperature (K)	Estimation Equation	Source Cited	Corresponding Section in Text
K_o	NA	cm/hr	NR	$1/K_o = 1/k_g + H/k_l$	See Section 4.3.2	
K_L	NA	NA	NR	$1/K_L = 1/k_l + 1/Hk_g$	See Section 4.3.2	
k_g	NA	NA		Eqs. 4-42, 4-43	See Section 4.3.2.1	
k_l	NA	NA		$k_l/U_w^* = a Sc^m$	Cohen and Ryan, 1985	4.3.2.2
D_{air}	0.096	cm ² /s	298.2	(a), Eq. 4-35	Cussler, 1984	4.3.1
D_{water}	1.02×10^{-5}	cm ² /s	298	(a), Eq. 4-37	Cussler, 1984	4.3.1
V_{d_B}	NA	NA	NR	Eq. 4-57	Cohen et al., 1990	4.3.3
$\tau_{1/2(air)}^{(t)}$	6.5 ± 1.95	days	298	(a)	Atkinson, 1989	4.4.1
$\tau_{1/2(water)}^{(t)}$	see Table 4-15 for measured values corresponding to specific conditions					4.4.2
$\tau_{1/2(oil)}^{(t)}$	see Table 4-15 for measured values corresponding to specific conditions					4.4.2

NR = Not Reported.

NA - The designation NA in the Units column indicates that the applicable correlations are in a dimensionless form or that any set of consistent units can be used.

Table 1-1. Summary of Representative Values or Estimation Equations for Required Input Parameters for Multimedia Assessment of Benzene
(Continued)

(a)	Measured value.
(b)	V_b at normal boiling point.
(c)	Measured value may vary with the soil type as well as the chemical composition of the soil organic carbon compounds.
(d)	Although measured values are available (Topp et al., 1989), they are highly dependent on experimental conditions, thus a general estimation equation for B_o has been provided.
(e)	Uncertainty in B_m and B_o estimated by McKone (1989) to be on the order of 2 orders of magnitude.
(f)	Reaction half-life.

3.1 Literature Review

A literature search of Dialog (NTIS, Pollution Abstracts, Enviroline) and UCLA Orion, Melvyl, and EMS library databases was conducted. The UCLA NCITR library was also reviewed for relevant publications. Through this process, references pertaining to the physicochemical properties, intermedia transport, and biotransformation of benzene were identified, obtained, reviewed, and summarized. Measured parameter values and estimation methods were evaluated and these are presented and discussed in the following sections.

3.2 Selection of Parameters

In order to provide an assessment of the pertinent intermedia transfer parameters, a number of input parameters were considered. Specifically, input parameters from the Air Resources Board/Department of Health Services (ARB/DHS) Health Risk Assessment (HRA) software and algorithms (CAPCOA Guidelines, 1990, 1991, 1992) and the South Coast Air Quality Management District Multi-Pathway Health Risk Assessment Input Parameters Guidance Document (SCAQMD, 1988) were considered. Three alternative multimedia models (SMCM, Fugacity, and GEOTOX) were also evaluated. The final selection was also based on the chemical and physical interpretation of the input parameters, their applicability to different classes of pollutants, and measures of the environmental consequences of intermedia transfers. The following subsections discuss the rationale for selecting input parameters as well as general limitations in their use.

3.2.1 Physicochemical Parameters

Physicochemical properties of benzene are needed for the determination of parameters such as partition coefficients and biotransfer factors, as well as for the analysis of intermedia transport parameters (e.g., mass transfer coefficients). Often the chemical properties that are needed are specific to the correlations that are used to evaluate factors such as partition coefficients and solubility.

The minimum necessary physicochemical factors for benzene required for conducting a multimedia exposure assessment of benzene as described by CAPCOA, 1992, and other models (i.e., SMCM, Fugacity, and GEOTOX) are as follows:

- Water Solubility;
- Vapor Pressure (as a function of temperature);
- Molar Volume (at the boiling point);
- Boiling Point; and
- Molecular Weight.

The definition of these parameters and the results of the literature review are presented in Section 4.1

3.2.2 Partition Coefficients

Benzene released to the environment is distributed to various environmental compartments as a result of transport processes. The net transport of benzene from one compartment to another is limited by equilibrium constraints and quantified by partition coefficients. Thus, the partition coefficient, H_{ij} is generally defined as

$$H_{ij} = C_i/C_j \quad (3-1)$$

where C_i is the equilibrium concentration in compartment i and C_j is the equilibrium concentration in compartment j . The following types of partition coefficients for benzene were considered in this study:

- Henry's Law Constant;
- Octanol-Water Partition Coefficient;
- Soil/Water-Organic Carbon Partition Coefficient;
- Bioconcentration Factors; and
- Biotransfer Factors.

Values for some partition coefficients for benzene reported in the literature have been determined experimentally in simulated ecosystems and estimated for others. These partition coefficients are discussed individually in Section 4.2.

3.2.3 Intermedia Transport Parameters

In order to estimate the rate of benzene transport across environmental phase boundaries, one must first be able to describe the transport mechanisms and consequently estimate the associated transport parameters as a function of the appropriate environmental conditions. The CAPCOA (1992) approach and other methodologies were reviewed and it was determined that the relevant intermedia transfer parameters for benzene are as follows:

- Diffusion Coefficients in Air and Water;
- Intermedia Mass Transfer Coefficients; and
- Deposition Velocity.

These intermedia transport parameters are defined and discussed in Section 4.3. In addition, bioavailability and pharmacokinetics considerations when evaluating benzene accumulation in biological receptors are briefly discussed in Section 4.2.6.

3.2.4 Degradation Processes

Reaction rates for individual abiotic and biotic degradation processes can be used to estimate overall environmental degradation half-lives. Degradation rates are determined for an individual chemical or biochemical transformation processes within specific media. Since degradation processes involve chemical changes as opposed to intermedia transport processes which involve the flux of the unchanged chemical through the environment, degradation half-lives for soil, water, and air do not account for intermedia transport of a chemical and are, therefore, not necessarily representative of a chemical's actual persistence within a particular environmental medium (Howard et al., 1991). Degradation processes

considered significant to assessing the transformation of benzene in the environment (Howard et al., 1991) are as follows:

Hydroxyl radical (OH) reaction in air: The most significant degradation process for benzene in the atmosphere is its reaction with atmospheric OH during daylight hours. Other potential degradation reactions include nighttime reaction with the gaseous nitrate (NO_3) radical and reaction of benzene with ozone. However, only the reaction of OH radicals is fast enough to be an important atmospheric loss process for benzene (see Section 4.4.1).

Biodegradation in water and soil: Biodegradation is one of the most important environmental processes that cause the breakdown of environmental compounds. It is a significant loss mechanism in soil and aquatic systems and plays an important role in wastewater treatment. The eventual mineralization of benzene - i.e., the complete conversion of benzene to inorganic substances (CO_2 and H_2O) - can be attributed almost entirely to biodegradation (Lyman et al., 1990). Bacteria are the most significant group of microorganisms involved in biodegradation. Soil, water, and wastewater treatment systems provide the most important habitats for the biodegradation of pollutants. In all three habitats both aerobic and anaerobic conditions exist. The half-lives reported in Howard et al. (1991) for aerobic conditions are considerably shorter than those for anaerobic conditions (ranging from 5 - 16 days to 4 - 24 months, respectively). Biodegradation rates of benzene in water and soil are higher under aerobic conditions so aerobic biodegradation is considered to be more important than anaerobic biodegradation.

Photolysis in air and water: Half-lives for direct photolysis are based on irradiation of a chemical in solution at environmentally important wavelengths (>290 nm). Photolysis rates in air are assumed to equal those in solution. The typical frequencies of maximum absorption, λ_{max} , and whether or not absorption occurs at wavelengths >290 nm may indicate whether a chemical has the potential to undergo photolysis in the environment. Measurements performed by Hustert (1981) in a solution of benzene and deionized water indicate that the photolysis half-life of benzene in water and air ranges from 117 to 673 days

(cited by Howard et al., 1991), which is too long to be considered significant when compared to biodegradation in water or reaction with OH radicals in air.

Photooxidation reactions with alkylperoxy (RO_2), hydroxyl radicals ($\text{OH}\cdot$) or singlet oxygen ($^1\text{O}_2$) in water: For some chemical classes, reactions with photooxidants in sunlit waters can be important. As with photooxidation in air by OH radicals, the range of half-lives is calculated from reaction rate constants and monitored concentrations of oxidants in relatively oligotrophic and eutrophic natural waters (Howard et al., 1991). Since the photooxidation half-life for benzene reported by Howard et al. (1991) is 36 years, this degradation process is not considered significant compared to biodegradation.

Hydrolysis in water and soil: Hydrolysis only applies to a limited number of chemicals that have hydrolyzable functional groups such as esters, aliphatic halogens, amides, carbamates, and phosphate esters. Since benzene does not contain hydrolyzable functional groups, hydrolysis is not a relevant degradation process.

In summary, the following abiotic and biotic degradation processes were evaluated for benzene:

- Reaction Rate/Half-Life in Air;
- Biodegradation Rate/Half-Life in Water; and
- Biodegradation Rate/Half-Life in Soil.

These processes are discussed further in Section 4.4.

4.0 PRESENTATION OF RESULTS

The following subsections define, discuss, and summarize the values and estimation methods for the benzene intermedia transfer factors reviewed in this study. Equations defining input parameters and estimation techniques are presented, where appropriate. A summary of the literature reported parameter values and estimation methods are

summarized in Tables 1-1 through 4-15. Data in the tables are arranged by decreasing order of reliability. Measured values of known uncertainty are listed first. Measured values reported without estimates of uncertainty are listed next, followed by calculated values reported with the corresponding prediction equations and uncertainty estimates. Calculated values reported without their associated estimation equations were reported last.

Values from references for which the derivation of the results could not be ascertained and multiple references to the same measured value are listed below the dotted line in the summary tables. The scientific confidence in these results is clearly limited; they have been included only to reflect the range of values commonly reported in the current environmental literature. Values for input parameters have been converted to consistent SI units to facilitate comparison of results. The converted values have been reported with same number of significant figures as the values reported in the corresponding reference. Specific conversion equations are shown in the tables. It should be noted that commonly used forms of estimation equations often require input parameters in non-SI units. These cases have been identified in the text following presentation of the appropriate equations.

4.1 Physicochemical Parameters

Section 3.2.1 describes the general need for using physicochemical parameters in multipathway assessment. This section defines the specific physicochemical parameters that should be used for multimedia analysis of pollutants and discusses the results of the literature survey. In general, the literature has sound measured values for these properties with little disagreement among results. One notable exception described, in Section 4.1.1, is the inaccurate solubility value that was reported by Hodgman (1952) and subsequently cited by some authors.

4.1.1 Solubility of Benzene in Water

The water solubility (S) of a chemical is defined as the maximum amount of the chemical that will dissolve in pure water at a specific pressure, temperature, and pH. The

units of aqueous solubility are usually stated in terms of weight per weight (ppm, ppb, g/kg, etc.) or weight per volume (mg/L, $\mu\text{g/L}$, mol/L, etc.). Less common units are mole fraction and molal concentration (moles per kg of solvent). In this report solubility is given in mol/L to be consistent with SI units. Values for the water solubility of benzene found in the literature are summarized in Table 4-1. Most solubility data were reported at 25° C.

Mackay and Shiu (1981) noted that many inaccurate data have been reported for solubility. For example, the Handbook of Chemistry and Physics (Hodgman, 1952) quoted the aqueous solubility of benzene as 800 g/m³ (0.01 mol/L) at 295 K. This value is approximately half the commonly reported value but has been quoted by Chiou et al. (1977) and is probably the source of the low solubility value attributed to Cheremisinoff and Morresi (1979) by CARB and CDHS (1984). The measured value reported by Seidell (1940) is also approximately half of the presently reported values and could not be reviewed for comparability since the reference was unavailable. Mackay and Shiu (1981) noted that the early data of McAuliffe (1966), who measured the solubility of benzene down to 1 ppm, have proved to be reliable and have been quoted by other researchers. Mackay concluded that the accepted value for water solubility for benzene was 1770 to 1780 g/m³ (0.0227 to 0.0228 mol/L) which is in agreement with the values presented in Table 4-1.

4.1.2 Vapor Pressure of Benzene as Cited in the Environmental Literature

The saturation vapor pressure, P_{vp} , is a measure of the volatility of a chemical in its pure state and is an important determinant of the rate of vaporization. Estimating P_{vp} requires information on the following properties: (1) critical temperature; (2) critical pressure; and (3) heat of vaporization, and/or the vapor pressure at some reference temperature. The units of P_{vp} can be stated in atm, torr, mm Hg, or Pa. In this report P_{vp} will be given in kPa.

Table 4-1. Solubility^(a) of Benzene in Water*

Solubility (mol/L)	Reported Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
0.0228	1780	ppm ^(b)	±45 ppm	298	Measured	McAuliffe, 1966	
0.0224 ^(c)	22,400	μM	±0.07	298	Measured	Banerjee et al., 1980	
0.0229 ^(d)	22.9	mol/m ³	NR	298	Measured	Miller et al., 1985	
0.0219 ^(e)	3.95 × 10 ⁻⁴	mole fraction	NR	298	Measured	Franks et al., 1963	
0.02247	1755	mg/L	NR	298	Measured	Mackay and Shiu, 1981; McAuliffe, 1966	McDevit and Long, 1952
0.02650	1769	mg/L	NR	298	Measured	Mackay and Shiu, 1981	Aquan-Yuen et al., 1979
0.0278	1779.5	mg/L	NR	298	Measured	Mackay and Shiu, 1981	Mackay and Shiu, 1975
0.0223	1740	mg/L	NR	298	Measured	Mackay and Shiu, 1981	Price, 1976
0.02393	1869	mg/L	NR	298	Measured	Mackay and Shiu, 1981	Klevens, 1950
0.023 ^(f)	1.79	g/L	NR	NR	Measured	Stephen and Stephen, 1963	Bohon and Claussen, 1951
0.0228	1740	mg/L	NR	NR	Measured	McAuliffe, 1966	Andrews and Keefer, 1949
0.02292	1790	mg/L	NR	NR	Measured	McAuliffe, 1966	Bohon and Claussen, 1951
0.0223	1740	mg/L	NR	NR	Measured	McAuliffe, 1966	Arnold et al., 1958
0.0222	1730	mg/L	NR	NR	Measured	McAuliffe, 1966	Franks et al., 1963
0.0186 ^(g)	1450	mg/L	NR	NR	Measured	McAuliffe, 1966 ^(h)	

Table 4-1. Solubility^(a) of Benzene in Water
(Continued)

Solubility (mol/L)	Reported Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
0.0092 ^(b)	0.072	weight %	NR	295	Measured	Stephen and Stephen, 1963	Seidell, 1940
0.013	1000	mg/L	NR	298	Measured	U.S. PHS, 1989	Krasnoshchekova and Gubergits, 1975
0.01780 ^(b)	1391	g/m ³	NR	298	Measured	Mackay and Shiu, 1975; Thibodeaux, 1979	
0.0227	1770	mg/L	NR	NR	Measured	Mackay and Shiu, 1981	NR
0.0228	0.0228	mol/L	NR	NR	NR	Kenaga and Goring, 1978	McAuliffe, 1966
0.0228	0.0228	mol/L	NR	NR	NR	Kenaga, 1980a	McAuliffe, 1966
0.0228 ^(b)	1780	µg/mL	NR	NR	NR	Cohen, 1989	McAuliffe, 1966
0.0228 ^(b)	1780	g/m ³	NR	NR	NR	Mackay and Leinonen, 1975; Mackay et al., 1980; Thibodeaux, 1979	McAuliffe, 1966
0.023	0.023	mol/L	NR	NR	NR	Verschueren, 1977	McAuliffe, 1966
0.023	2.3 × 10 ⁻²	mol/L	NR	NR	NR	McKone and Layton, 1986	McAuliffe, 1966

Table 4-1. Solubility^(a) of Benzene in Water^{*}
(Continued)

Solubility (mol/L)	Reported Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
0.0229 ^(b)	$1 \times 10^{-1.64}$	mol/L	NR	NR	NR	Chiou and Schmedding, 1982; Chiou et al., 1983; Chiou, 1985	McAuliffe, 1966
0.010 ^(c)	0.072	ppm ^(b)	NR	295	NR	Chiou et al., 1977	Hodgman, 1952
0.011 ^(c)	0.82	mg/g	NR	NR	NR	CARB and CDHS, 1984	Cheremisinoff and Morresi, 1979 ^(b)
0.0228	22.8	mol/m ³	NR	293	NR	Hattemer-Frey and Travis, 1990; Wakeham et al., 1986	Wakeham et al., 1986; Hovrath, 1982; Mabey et al., 1981

NR = Not reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) The water solubility of a chemical is defined as the maximum amount of the chemical that will dissolve at a specific temperature and pH.

(b) Parts per million (ppm) equivalent to µg/mL in aqueous solutions, thus conversion factor same as in footnote (h) below.

(c) Conversion from reported value: $22400 \mu\text{M} \times \frac{1 \text{ mol benzene}}{10^6 \mu\text{mol}} = 0.0224 \text{ mol/L}$
where M = mol/L

(d) Conversion from reported value: $22.9 \frac{\text{mol}}{\text{m}^3} \times \frac{1 \text{ m}^3}{1000 \text{ L}} = 0.0229 \text{ mol/L}$

Table 4-1. Solubility^(a) of Benzene in Water^{*}
(Continued)

(e)	Conversion from reported value: $3.95 \times 10^{-4} \frac{\text{mol benzene}}{\text{mol water}} \times \frac{1 \text{ mol water}}{18 \text{ g water}} \times \frac{1000 \text{ g water}}{1 \text{ t water}} = 0.0219 \text{ mol/L}$
(f)	Conversion from reported value: $1.79 \text{ g/L} \times \frac{1 \text{ mol benzene}}{78.1 \text{ g benzene}} = 0.023 \text{ mol/L}$
(g)	Conversion from reported value: $1450 \text{ mg/L} \times \frac{1 \text{ mol benzene}}{78.1 \text{ g benzene}} \times \frac{1 \text{ g}}{1000 \text{ mg}} = 0.0186 \text{ mol/L}$
(h)	Conversion from reported value: $1780 \text{ } \mu\text{g/mL} \times \frac{1 \text{ mol benzene}}{78.1 \text{ g benzene}} \times \frac{1 \text{ g}}{10^6 \text{ } \mu\text{g}} \times \frac{1000 \text{ mL water}}{1 \text{ L water}} = 0.0228 \text{ mol/L}$
(i)	Conversion from reported value: $0.072\% \frac{\text{g benzene}}{\text{g water}} \times \frac{1 \text{ mol benzene}}{78.1 \text{ g benzene}} \times \frac{1000 \text{ g water}}{1 \text{ t water}} \times \frac{1}{100\%} = 0.0092 \text{ mol/L}$
(j)	Solubility of benzene in seawater matrix.
(k)	Conversion from reported value: $1780 \text{ g/m}^3 \times \frac{1 \text{ mol benzene}}{78.1 \text{ g benzene}} \times \frac{1 \text{ m}^3 \text{ water}}{1000 \text{ L water}} = 0.0228 \text{ mol/L}$
(l)	Conversion from reported value: $10^{-1.64} \text{ mol/L} = 0.0229 \text{ mol/L}$
(m)	Value considered inaccurate, see Section 4.1.1.
(n)	Conversion from reported value: $0.82 \frac{\text{mg}}{\text{g}} \times \frac{1 \text{ mol benzene}}{78.1 \text{ g}} \times \frac{1 \text{ g}}{1000 \text{ mg}} \times \frac{1000 \text{ g}}{1 \text{ t}} = 0.011 \text{ mol/L}$

The vapor pressure of benzene is dependent on temperature and it can be calculated from the following Antoine equation (Zwolinski and Wilhoit, 1971)¹:

$$\log_{10} P_{vp} = A - B/(C + T) \quad (4-1)$$

where P_{vp} is the vapor pressure (mm Hg); T is the temperature (K), and where the constants of the Antoine Equation for benzene are given as:

$$A = 6.90565$$

$$B = 1211.033$$

$$C = - 52.36$$

The above equation is applicable only for a temperature range of 288 K to the critical temperature of benzene (562.2 K).

Examples of vapor pressures reported in the literature for benzene are listed in Table 4-2. The P_{vp} values were generally calculated at standard conditions (298 K) and ranged from 12.6 to 12.7 kPa. The small difference observed is probably due to rounding of the Antoine equation coefficients. At 293 K, the experimental value for P_{vp} is 10 kPa. Lyman et al. (1990) discuss the calculation of P_{vp} by using the Antoine Equation and compare the measured value with the calculated result. Lyman et al. (1990) reported that the Antoine equation is applicable over the pressure range from 10^{-3} to 760 mm Hg. However, Reid et al. (1977) suggest that this equation may not be suitable for estimating pressures below about 10 mm Hg.

4.1.3 Molar Volume of Benzene

The molar volume (V_b) of benzene, expressed in units of cm^3/mol , is the volume of a mole of liquid benzene at the normal boiling temperature. The molar volume of an

¹ The value of the constant C as given in the original reference was modified to correspond to the change of the temperature scale to degrees Kelvin.

Table 4-2. Vapor Pressure of Benzene as Cited in the Environmental Literature*

Vapor Pressure (kPa)	Reported Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
10 ^(a)	76	mm Hg	NR	293	Measured	Lyman et al., 1990	Balson, 1947; Goring and Hanamaker, 1972; Stull, 1947; Yaws, 1977
12.7	12.7	kPa	NR	NR	Calculated	Mackay and Shiu, 1981	Zwolinski and Wilhoit, 1971
12.7 ^(a)	95.2	mm Hg	NR	NR	Calculated	Mackay and Wolkoff, 1973	Zwolinski and Wilhoit, 1971
12.7 ^(b)	95.18	torr	NR	298	Calculated	U.S. PHS, 1989	Zwolinski and Wilhoit, 1971
12.7 ^(c)	12,700	Pa	NR	NR	NR	Mackay and Paterson, 1988	Mackay et al., 1981
12.6 ^(b)	95	torr	NR	NR	NR	McKone and Layton, 1986	Layton et al., 1986 ^(c)
12.6 ^(d)	0.125	atm	NR	298	NR	U.S. PHS, 1989	Thibodeaux, 1981
10 ^(b)	75	torr	NR	NR	NR	Layton et al., 1986	Verschueren, 1983
13 ^(a)	100	mm Hg	NR	299.1	NR	IARC, 1982	Weast, 1979
6.051 ^(b)	45.53	torr	NR	283	NR	U.S. PHS, 1989	Zwolinski and Wilhoit, 1971
24.29 ^(b)	182.8	torr	NR	310	NR	U.S. PHS, 1989	Zwolinski and Wilhoit, 1971
12 ^(c)	87 ^(f)	mm Hg	NR	310-449	Calculated ^(f)	CARB and CDHS, 1984	Perry and Chilton, 1973
12.7 ^(a)	95.2	mm Hg	NR	NR	NR	U.S. EPA, 1987	NR

Table 4-2. Vapor Pressure of Benzene as Cited in the Environmental Literature*
(Continued)

Vapor Pressure (kPa)	Reported Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
12.7 ^(a)	95.2	mm Hg	NR	NR	NR	Mackay and Leinonen, 1975	NR
12.6 ^(d)	0.125	atm	NR	298	NR	Thibodeaux, 1979	NR
10 ^(d)	0.1	atm	NR	293	NR	Mackay and Yeun, 1983	NR

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) Conversion from reported value: $\text{mmHg} \times \frac{1 \text{ atm}}{760 \text{ mmHg}} \times \frac{101 \text{ kPa}}{1 \text{ atm}} = \text{kPa}$

(b) Conversion from reported value: $\text{torr} \times \frac{1 \text{ atm}}{760 \text{ torr}} \times \frac{101 \text{ kPa}}{1 \text{ atm}} = \text{kPa}$

(c) Conversion from reported value: $\text{Pa} \times \frac{1 \text{ kPa}}{1000 \text{ Pa}} = \text{kPa}$

(d) Conversion from reported value: $\text{atm} \times \frac{101 \text{ kPa}}{1 \text{ atm}} = \text{kPa}$

(e) Cited reference determined as per Dr. T. McKone (Lawrence Livermore National Laboratory).

(f) Reported value determined from the following equation: $\ln P = -4033 \times \frac{1}{T} + 18$, mm Hg (T in K)

organic liquid is a useful parameter because it has been correlated with the normal boiling point and it is used in techniques for estimating diffusion coefficients in air and water.

The molar volume of benzene is presented in Table 4-3. Of the two measured values presented, the value of 96.5 cm³/mol (Lee et al., 1973) is considered more accurate since it agrees with the calculated values determined by three different estimation techniques (e.g., the methods of LeBas, 1915 and Schroeder, 1949). The measured value of Chiou et al. (1983) (89.4 cm³/mol) was within 7.6% relative percent difference of the Lee et al. (1973) value.

4.1.4 Boiling Point Temperature of Benzene

The boiling point temperature, T_{BP} , is defined as the temperature at which the vapor pressure of a liquid is equal to the total pressure above the liquid. For pure compounds, the normal T_{BP} is defined as the T_{BP} at one standard atmosphere of pressure on the liquid. T_{BP} provides an indication of the physical state and volatility of a chemical. T_{BP} can be also an important parameter used in the prediction of other physical properties such as the enthalpy of vaporization.

Examples of boiling points reported in the literature for benzene are listed in Table 4-4. If one applies the standard pressure of 760 mm Hg to Eq. 4-1, then the calculated boiling point temperature for benzene would be:

$$T_{BP} = B/(A - \log_{10}P_s) - C \quad (4-2)$$

in which $P_s = 760$ mm Hg and thus $T_{BP} = 353.25K$ which agrees with the values reported in Table 4-4.

Table 4-3. Molar Volume^(a) (V_b) of Benzene*

Value (cm ³ /mol)	Reported Value	Reported Units	Reported Uncertainty (% error)	Temperature (K)	Technique	Reference	Source Cited
96.5	96.5	cm ³ /mol	NR	(b)	Measured	Reid et al., 1987	Lee et al., 1973
89.4	0.0894	L/mol	NR	(b)	Measured	Chiou et al., 1983	
96.5	96.5 ^(c)	cm ³ /mol	NR	(b)	Measured	Reid et al., 1977	Lee et al., 1973
96.4	96.4	cm ³ /mol	-0.1	(b)	Calculated ^(d)	Reid et al., 1987	
98	98.0	cm ³ /mol	1.6	(b)	Calculated ^(e)	Reid et al., 1987	Schroeder (in Partington, 1949)
96	96.0	cm ³ /mol	-0.5	(b)	Calculated	Reid et al., 1987	Le Bas, 1915
88.7	88.7	cm ³ /mol	NR	(b)	NR	Miller et al., 1985	NR

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) Molar volume is the volume of a mole of a liquid at the normal boiling temperature.

(b) At normal boiling point.

(c) Molal volume.

(d) $V_b = 0.285 V_c^{1.048}$; V_c = critical volume (cm³/mol).

(e) Additive method based on number of atoms and double bond (Reid, 1987).

Table 4-4. Examples of Boiling Point Temperature (T_{BP}) Reported in the Literature for Benzene* (a)

Boiling Point (K)	Reported Value	Reported Units	Reported Uncertainty	Conditions	Technique	Reference	Source Cited
353 ^(b)	80.1	°C	NR	760 mm Hg	NR	U.S. PHS, 1989	Weast et al., 1985
353 ^(c)	176	°F	NR	1 atm	NR	CARB and CDHS, 1984	Perry and Chilton, 1973
353 ^(b)	80.1	°C	NR	NR	NR	IARC, 1982	NR
353 ^(b)	80.1	°C	NR	NR	NR	Mackay and Shiu, 1981	NR
353 ^(b)	80.1	°C	NR	NR	NR	Weast et al., 1985	NR

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) See section 4.1.4 for the Antoine equation used to calculate the boiling point.

(b) Conversion from reported value: $80.1^{\circ}\text{C} + 273 = 353\text{K}$

(c) Conversion from reported value: $\frac{176^{\circ}\text{F} - 32}{1.8} + 273 = 353\text{K}$

4.1.5 Molecular Weight of Benzene

The molecular weight is used for converting from mass to concentration and in various correlations of transport properties (e.g., diffusion coefficients). The molecular weight of benzene is 78.114 g/mol, exactly as accepted by IUPAC (IUPAC, 1987; cited by Buldavari et al., 1989). The values varied from 78 to 78.114. The only differences being in the number of significant figures reported or rounding to significant figures.

4.2 Partition Coefficients

Section 3.2.4 provides general equations for the various partition coefficients. The definitions and findings of the literature search for the individual partition coefficients and are presented in the following subsections.

4.2.1 Henry's Law Constant for Benzene

The Henry's Law constant is a particularly important parameter for evaluating chemical partitioning between air and water and is required as an input parameter in most multimedia models. In most situations, benzene concentrations in water are very small and Henry's Law is applicable. Henry's Law constant of a chemical (H_i) is defined as:

$$H_i = P_i / C_i \quad (4-3)$$

where P_i is the partial pressure of the contaminant (e.g., Pa units) at the system temperature, and C_i is the concentration (e.g., mol/m³) of the chemical in the aqueous phase in equilibrium with the air phase. The Henry's Law constant may be determined experimentally or estimated. However, it is preferable to use an experimentally determined value since they are generally more reliable than estimated values. An estimated value of H_i can be obtained by using the saturation vapor pressure and solubility data in the following equation (Lyman et al., 1990 and Reid et al., 1987):

$$H_i = P_{vp}/S \quad (4-4)$$

where S is the aqueous phase solubility (e.g., mol/m³) and P_{vp} is the saturation vapor pressure of the compound (e.g., Pa). This expression is valid only when the solute activity coefficient is constant for the concentration range up to the solubility limit. Since this assumption is not valid in most cases, Eq. 4-4 should only be regarded as an approximation. It should also be noted that Henry's Law constant is temperature dependent and for benzene it can be estimated from the empirical correlation of Leighton and Calo (1981),

$$H' = [0.21935 \exp(19.02 - 3964/T)] / T \quad (4-5)$$

where $H' = H_i/RT$, is the dimensionless Henry's Law constant, T is the temperature in K, and R is the gas constant ($R = 8.205 \times 10^{-5}$ atm·m³/g mol).

Table 4-5 presents Henry's Law constants for benzene at various temperatures which range from 0.324 to 0.555 kPa m³/mol. Mackay et al. (1979) critically reviewed Henry's Law constants for 150 hydrophobic compounds and recommended a Henry's Law constant of 0.550 ± 0.025 kPa m³/mol for benzene; the recommended value encompasses the range of measured values (at 298 K) as presented in Table 4-5.

4.2.2 Octanol-Water Partition Coefficient for Benzene

The octanol-water partition coefficient, K_{ow} , is defined as the equilibrium ratio of the concentration of a chemical in the octanol phase to its concentration in the aqueous phase of a two-phase octanol/water system by the following equation:

$$K_{ow} = C_o/C_w \quad (4-6)$$

where C_o is the concentration in octanol phase and C_w is the concentration in aqueous phase.

Table 4-5. Henry's Law Constant (H) for Benzene*

Henry's Law Constant (kPa m ³ /mol)	Reported Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
0.555	0.555 ^(a)	kPa m ³ /mol	±6%	298	Measured	Mackay et al., 1979	
0.324	3200	atm cm ³ /mol	NR	288	Measured	Chiang et al., 1989	Kavanaugh and Trussell, 1980
0.550	0.550	kPa m ³ /mol	±0.025	298	Calculated	Mackay and Shiu, 1981	
0.439 ^(b)	3300	torr kg/mol	NR	293	Calculated ^(c)	Layton et al., 1986	NR
0.554 ^(d)	5.49×10 ⁻³	atm m ³ /mol	NR	NR	Calculated	Mackay and Shiu, 1975	
0.44 ^(e)	0.185	dimensionless	NR	293	Calculated	Cohen and Ryan, 1989	Leighton and Calo, 1981
0.55 ^(d)	0.0055	atm m ³ /mol	NR	298	NR	CARB and CDHS, 1984	Thibodeaux, 1979
0.554 ^(d)	5.49×10 ⁻³	atm m ³ /mol	NR	NR	NR	Thibodeaux, 1979	Mackay and Shiu, 1975
0.55 ^(d)	5.5×10 ⁻³	atm m ³ /mol	NR	NR	NR	U.S. PHS, 1989	Mackay and Leinonen, 1975
0.55 ^(d)	5.5×10 ⁻³	atm m ³ /mol	NR	293	NR	Wakeham et al., 1986	Mackay and Shiu, 1981
0.55 ^(d)	5.5×10 ⁻³	atm m ³ /mol	NR	NR	NR	Mackay and Leinonen, 1975	NR
0.55 ^(d)	5.5×10 ⁻³	atm m ³ /mol	NR	NR	NR	Hattemer-Frey and Travis, 1990	Lyman et al., 1982
0.442 ^(d)	4.39×10 ⁻³	atm m ³ /mol	NR	293	NR	Mackay and Yeun, 1983	NR
0.549 ^(b)	4130	torr kg/mol	NR	NR	NR	McKone and Layton, 1986	NR
0.439 ^(d)	3300	torr L/mol	NR	NR	NR	McKone, 1988	NR

Table 4-5. Henry's Law Constant (H) for Benzene*
(Continued)

Henry's Law Constant (kPa m ³ /mol) Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
0.44 ^(b)	dimensionless	NR	293	NR	Cohen and Ryan, 1989	Rogers et al., 1980
0.534 ^(b)	dimensionless	NR	NR	NR	Jury et al., 1984	NR

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) Based on the formula, $H = P_{vp} \times MW/S$, the authors reported 8 estimated Henry's Law constants ranging from 0.533 to 0.570 and recommended a value of 0.550 ± 0.025 .

(b) Conversion from reported value: $\text{torr} \cdot \frac{\text{kg}}{\text{mol}} \times \frac{1 \text{ atm}}{760 \text{ torr}} \times \frac{101 \text{ kPa}}{1 \text{ atm}} \times \frac{10^{-3} \text{ m}^3}{1 \text{ kg}} = \text{kPa m}^3/\text{mol}$

(c) Calculated by dividing vapor pressure by solubility.

(d) Conversion from reported value: $\text{atm m}^3/\text{mol} \times \frac{101 \text{ kPa}}{1 \text{ atm}} = \text{kPa m}^3/\text{mol}$

(e) Calculated from Eq. (4-5), see footnote (h) for conversion of dimensionless Henry's Law constant to units of kPa m³/mol.

(f) Conversion from reported value: $\text{torr} \cdot \frac{\text{L}}{\text{mol}} \times \frac{1 \text{ atm}}{760 \text{ torr}} \times \frac{101 \text{ kPa}}{1 \text{ atm}} \times \frac{10^{-3} \text{ m}^3}{1 \text{ kg}} \times \frac{1 \text{ kg}}{1 \text{ L}} = \text{kPa m}^3/\text{mol}$

(g) Reported as $H_{\text{m}} = C_v/C_g$; conversion from reported value is as follows: $H = 1/H_{\text{m}}$

(h) Conversion from reported value: $H(\text{dimensionless}) \times RT = H(\text{kPa m}^3/\text{mol})$
 $R = (82.05 \text{ atm cm}^3/\text{K mol}) \times \frac{101 \text{ kPa}}{1 \text{ atm}} \times \frac{1 \text{ m}^3}{1 \times 10^6 \text{ cm}^3}; T = 293 \text{ K}$

When the concentrations of C_o and C_w are in the same units (e.g., mol/cm³), values for K_{ow} are unitless. K_{ow} is an important parameter used in the assessment of environmental fate and transport for organic chemicals because the octanol phase is a surrogate for the lipid phase or organic carbon content of environmental compartments. Since K_{ow} has been correlated to water solubility, soil/sediment adsorption coefficients, and bioconcentration factors for aquatic life (Lyman et al., 1990), it is a key variable used in the estimation of these properties. Although K_{ow} is expected to vary with temperature, its temperature dependence is rarely reported.

Table 4-6 presents log K_{ow} values for benzene. Five measured values found in literature were determined at various temperature. Only two of these values were determined at the same temperature (298K). The value of 2.13 for log K_{ow} reported by Fujita et al. (1964) is considered the most reliable because it is associated with a calculated uncertainty of ± 0.01 log K_{ow} units and it is the value most commonly cited in the literature. The validity of this value was confirmed by Miller et al. (1985) who also obtained a value of 2.13 for K_{ow} .

4.2.3 Soil/Water-Organic Carbon Coefficient for Benzene

The organic carbon partition coefficient (K_{oc}) is a measure of the tendency for organics to adsorb onto the soil (or sediment) and is defined as the ratio of the amount (mass) of a chemical adsorbed per unit mass of organic carbon in the soil or sediment to the concentration of the chemical in the soil (or sediment) solution at equilibrium,

$$K_{oc} = \frac{(\text{mg chemical adsorbed/kg organic carbon})}{\text{mg chemical dissolved/l of solution}} \quad (4-7)$$

The available methods for estimating K_{oc} involve empirical relationships with other properties of a chemical such as solubility, octanol-water partition coefficient, or bioconcentration factor for aquatic life. Lyman et al. (1990) recommends the following estimation correlations for aromatic compounds (e.g., benzene).

Table 4-6. Octanol-Water Partition Coefficient ^(a)(K_{ow}) for Benzene*

log K _{ow} (dimensionless)	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
2.13	± 0.01 (log K _{ow})	298	Measured	Leo et al., 1971; Chiou et al., 1977; Mackay et al., 1980; Chiou and Schmedding, 1982; Chiou et al., 1983; Chiou, 1985; Hattermer-Frey and Travis, 1990; U.S. PHS, 1989	Fujita et al., 1964
2.12	± 1.2% (K _{ow})	296	Measured	Banerjee et al., 1980	
2.14				CARB & CDHS, 1984	Cheremisinoff and Morris, 1979
2.12	NR	293	Measured	Veith et al., 1980	
2.13	NR	298	Measured	Mackay and Paterson, 1988	Miller et al., 1985
2.13				Layton et al., 1986; McKone and Layton, 1986; McKone, 1989	Verschueren, 1983
2.11	NR	NR	Measured	Karickhoff et al., 1979	
1.90	NR	NR	Calculated ^(b)	Mackay et al., 1980	
2.13	NR	NR	Calculated ^(c)	Veith et al., 1980	Veith and Morris, 1979

Table 4-6. Octanol-Water Partition Coefficient ^(a)(K_{ow}) for Benzene*
(Continued)

log K _{ow} (dimensionless)	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
2.13	±0.15 (log K _{ow})	NR	Calculated	Veith et al., 1980	Leo, 1978
2.13	NR	NR	NR	Wakeham et al., 1986	Hansch and Leo, 1979
2.12	NR	NR	NR	U.S. EPA, 1987	NR
1.56	NR	NR	NR	Leo et al., 1971; U.S. PHS, 1989	Rogers and Cammarata, 1969
2.15	NR	NR	NR	Leo et al., 1971; U.S. PHS, 1989	Private Communication

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) Octanol-water partition coefficient (K_{ow}) is defined as the ratio of the concentration of a chemical in the octanol phase to its concentration in the aqueous phase in a two-phase octanol/water system. Values for K_{ow} are dimensionless.

(b) $\ln K_{ow} = 7.494 - \ln S$, where S equals water solubility.

(c) Estimated using reverse-phase liquid chromatography; $\log K_{ow} = 5.106 \log RT - 1.258$; RT is the chromatographic retention time.

$$\log K_{oc} = -0.54 \log S + 0.44 \quad (\text{Karickhoff et al., 1979}) \quad (4-8)$$

where S is the aqueous chemical solubility expressed in units of mole fraction.

$$\log K_{oc} = 1.00 \log K_{ow} - 0.21 \quad (\text{Karickhoff et al., 1979}) \quad (4-9)$$

$$\log K_{oc} = 0.937 \log K_{ow} - 0.006 \quad (\text{Brown et al., 1990 as cited by Lyman et al, 1990}) \quad (4-10)$$

The results in Table 4-7 show a wide range of values for K_{oc} reported in the literature. Differences in measured values are attributed to the dependence of K_{oc} on soil characteristics such as pore size distribution, moisture content, pH, and soil chemistry. The variability of the calculated values is attributed to the use of different estimation equations as previously described.

4.2.4 Bioconcentration Factors for Benzene

The traditional measure of a chemical's potential to accumulate in an organism is the bioconcentration factor (BCF), which is defined as a chemical's wet-weight concentration in an organism or tissue divided by its concentration in the medium through which exposure occurs by direct contact (e.g., water for aquatic organisms, or air for terrestrial organisms). The concept of BCF addresses partitioning of a chemical into an organism by non-food routes. Specifically, BCF is defined as:

$$BCF = \frac{(\text{equilibrium concentration of chemical in receptor})}{(\text{mean concentration of chemical in the medium through which exposure occurs by direct contact})} \quad (4-11)$$

It is convenient to use the same units for both the numerator and denominator which results in a dimensionless BCF. The term BCF is used with the assumption that uptake across external membranes from the media with which the receptor is in direct contact is the chief pathway for chemical uptake by the organism. Table 4-8 presents benzene BCF

Table 4-7. Soil/Water-Organic Carbon Coefficient (K_{oc})^(a) for Benzene*

Value (b)	Reported Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
83	83	dimensionless	NR	NR	Measured	Kenaga, 1980 Howard et al., 1987	Kenaga and Goring, 1978
31	31	dimensionless	NR	NR	Measured	Chiou et al., 1983	Chiou et al., 1983
537	2.73	log K_{oc}	NR	NR	Measured ^(c)	Urchin and Mangels, 1987	
338	2.53	log K_{oc}	NR	NR	Measured ^(c)	Urchin and Mangels, 1987	
144	2.16	log K_{oc}	NR	NR	Measured ^(c)	Urchin and Mangels, 1987	
1023	3.01	log K_{oc}	NR	NR	Measured ^(c)	Urchin and Mangels, 1987	
204	2.31	log K_{oc}	NR	NR	Measured ^(c)	Urchin and Mangels, 1987	
123	2.09	log K_{oc}	NR	NR	Measured ^(c)	Urchin and Mangels, 1987	
83	83	dimensionless	NR	298	Measured	Kenaga and Goring, 1980	Karickhoff et al., 1979
71	71	dimensionless	± 1.2 (Orders of Magnitude)	NR	Calculated ^(d)	Kenaga, 1980	Kenaga and Goring, 1978
76	76	dimensionless	NR	NR	Calculated	Layton et al., 1986	Karickhoff et al., 1979
98	98	dimensionless	NR	NR	Calculated ^(e)	Howard et al., 1987	Lyman et al., 1982
63 ^(f)	1.8 ^(g)	L/kg _{oc}	NR	NR	Calculated ^(h)	Wakeham, 1986	Chiou et al., 1979
84	84	mL/g	NR	NR	NR	Hattener-Frey and Travis, 1990	Lyman et al., 1982
83	83	dimensionless	NR	NR	NR	U.S. EPA, 1987	NR
48	48	dimensionless	NR	NR	NR	McKone and Layton, 1986	NR

Table 4-7. Soil/Water-Organic Carbon Coefficient (K_{oc})^(a) for Benzene*
(Continued)

Value (b)	Reported Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
76	76	dimensionless	NR	NR	NR	McKone, 1988	NR
0.3-100	0.3-100	NR	NR	NR	NR	U.S. PHS, 1989	Rogers et al., 1980
31.7-143	31.7-143	dimensionless	NR	NR	NR	Howard et al., 1987	Sabljic, 1984

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) Organic carbon partition coefficient (K_{oc}) is defined as the ratio of the mass of a chemical adsorbed per unit mass of organic carbon in the soil or sediment to the concentration of the chemical in the solution at equilibrium.

(b) Units for K_{oc} determined as follows:

$$K_{oc} = \frac{\mu\text{g adsorbed/g organic carbon}}{\mu\text{g/mL solution}} \quad K_{oc} = \frac{\text{mL solution}}{\text{g organic carbon}}$$

recommended correlations (Lyman et al., 1990)

$$\log K_{oc} = -0.54 \log S + 0.44; \quad S \text{ in units of mole fraction} \quad \log K_{oc} = 1.00 \log K_{ow} - 0.21 \quad \log K_{oc} = 0.937 \log K_{ow} - 0.006$$

(c) Measured in 2 types of aquifer solids with 2.6 and 1.3% OC content for 3 different adsorbent masses (1, 5, 10g).

(d) Calculated using equation of Kenaga and Goring, 1978: $\log K_{oc} = 3.64 - 0.55 (\log S)$, where S is water solubility (ppm). Uncertainty in the predictions of this equation was estimated to be ± 1.23 orders of magnitude for the 95% confidence interval.

(e) Based on $K_{ow} = 2.13$; $\log K_{oc} = 0.937 \log K_{ow} - 0.006$ (Lyman, 1982).

(f) Calculated as the inverse log of 1.8.

(g) $\log K_{oc}$ calculated using equation by Chiou et al., 1979; $\log K_{oc} = -0.557 \log S + 4.277$, where S equals water solubility in $\mu\text{mol/L}$.

(h) Soil-organic matter coefficient (K_{om}) measured as Woodburn silt loam (1.9% organic matter); K_{oc} calculated as 1.72 (K_{om}).

Table 4-8. Bioconcentration Factor (BCF)^(a) for Benzene in Aquatic Organisms*

Bioconcentration Factor ^(b) (dimensionless)	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
3.5 ^(c)	NR	NR	Measured	Howard et al., 1987	Ogata and Miyake, 1978
4.4 ^(d)	NR	NR	Measured	Howard et al., 1987	Kom et al., 1977
4.3 ^(e)	NR	NR	Measured	Howard et al., 1987	Ogata et al., 1984
9	+2 orders of magnitude in the 95% confidence limit	NR	Calculated ^(f)	Kenaga, 1980	Kenaga and Goring, 1978
3	±1.95 orders of magnitude in the 95% confidence limit	NR	Calculated ^(g)	Kenaga, 1980	Kenaga and Goring, 1978
25	NR	NR	Calculated ^(h)	Layton et al., 1986	Layton et al., 1986
19	NR	NR	Calculated	McKone and Layton, 1986	Kenaga and Goring, 1978
24	NR	NR	Calculated ^(b)	Howard et al., 1987	Lyman et al., 1982
25	NR	NR	Calculated	McKone, 1988	NR
<hr/>					
5.2	NR	NR	NR	Hattemer-Frey and Travis, 1990	U.S. EPA, 1986a
5.2	NR	NR	NR	U.S. EPA, 1987	NR

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

Table 4-8. Bioconcentration Factor (BCF)^(a) for Benzene in Aquatic Organisms*
(Continued)

(a)	The bioconcentration factor (BCF) is the concentration of a chemical in an organism divided by the concentration in water.
(b)	BCF in fish, unless otherwise noted.
(c)	Eels.
(d)	Pacific Herring.
(e)	Goldfish.
(f)	Calculated from solubility; $\log \text{BCF} = 2.791 - 0.564 (\log S)$, where S is aqueous solubility (mol/L).
(g)	Calculated from soil/organic carbon coefficient, K_{oc} ; $\log \text{BCF} = -1.579 + 1.119 (\log K_{oc})$.
(h)	Calculated as $\log \text{BCF} = 0.76 \log K_{ow} - 0.23$.

values for fish (species unknown unless footnoted). It is important to note that BCF values are compound-specific, medium-specific, and species-specific, and experimental data should be used whenever possible. In the absence of data, various empirical correlations may be utilized to estimate BCF values. Several log BCF - log K_{ow} correlations, specific to benzene derivatives are given below:

$$\log \text{BCF} = 0.206 + 0.6669 \log K_{ow} \quad (\text{Lu, 1974}) \quad (4-12a)$$

$$\log \text{BCF} = 0.76 \log K_{ow} - 0.23 \quad (\text{Veith et al., 1980}) \quad (4-12b)$$

$$\log \text{BCF} = 0.935 \log K_{ow} - 1.495 \quad (\text{Kenaga and Goring, 1980}) \quad (4-12c)$$

Eq. 4-12a was derived from model ecosystem tests which tend to underestimate BCFs since equilibrium conditions may not have been established (Lyman et al., 1990). Eqs. 4-12b and 4-12c were derived from data based on well-mixed flow through systems that are more reliable because efficient mass transfer and thus equilibrium accumulation is more likely to be achieved.

Bioconcentration in Vegetation

The concept of BCFs has also been applied to root uptake and air-to-leaf pathways. The accumulation of benzene in vegetation is a complex process that can involve deposition, root uptake, and air-to-leaf transfer. Volatile organics such as benzene are not expected to partition to any significant extent onto atmospheric aerosols (Bidleman, 1988). Thus, benzene is present in the environment in its primary gaseous and dissolved forms. Therefore, it can be assumed that contamination of plants by direct deposition of particles onto which benzene is adsorbed is not a significant exposure pathway.

Pollutants can accumulate in vegetation through the uptake of contaminated water from the soil. However, benzene is not very soluble in water, so root uptake is not expected to be a major source of vegetative contamination. The concentration of benzene in vegetation due to root uptake (C_v) has been estimated by (Topp et al., 1989) as

$$C_{vr} = C_s B_{vd} \quad (4-13)$$

where C_s is the concentration of benzene in soil (e.g., ng chemical/kg soil) and B_{vd} is a benzene-specific bioconcentration factor determined on a dry-weight basis.

$$B_{vd} = \frac{(\text{concentration of benzene in plant})}{(\text{concentration of benzene in soil})} \quad (4-14a)$$

where the concentration in the plant, C_{vr} , is based on dry mass (e.g., ng chemical/kg dry plant). Travis and Arms (1988) proposed the following correlation for the above-ground portion of the plant bioconcentration factor, B_{vd} :

$$\log B_{vd} = 1.588 - 0.5781 \log K_{ow} \quad r^2 = 0.525 \quad (4-14b)$$

If B_{vw} values based on wet weight are desired, then the dry weight values can be converted to a wet weight basis using soil density (or moisture content and the wet weight of the plant). For example, Briggs et al. (1982) proposed the following definition for the root bioconcentration factors for root crops:

$$B_{vw} = \frac{C_{veg}}{C_{soil}} \quad (4-15)$$

in which C_{veg} is the chemical concentration in the wet plant (e.g., ng chemical/kg plant). Thus, B_{vw} is related to B_{vd}

$$B_{vw} = B_{vd} \times f_{dw} \quad (4-16)$$

where f_{dw} is the fraction of dry plant matter in the wet plant. Briggs et al. (1982) proposed the following correlation for B_{vw} :

$$B_{vw} = \frac{0.82 + 0.028 K_{ow}^{0.77}}{K_d} \quad (4-17)$$

in which $K_d = K_{oc} \chi$ where χ represents the mass fraction of the soil natural organic carbon.

Air-to-leaf transfer is considered a key pathway for the uptake of benzene, from the atmosphere by vegetation. The concentration of a chemical in vegetation due to air-to-leaf transfer, C_v (e.g., ng/kg dry plant) can be estimated from the plant-air bioconcentration factor (Hattemer-Frey and Travis, 1990)

$$B_{vaw} = \frac{C_v \rho_p}{C_a F_v} \quad (4-18)$$

where C_a is the concentration of a chemical in the air (e.g., $\mu\text{g}/\text{m}^3$), F_v represents the fraction of a chemical in the vapor phase, ρ_p is the fresh plant density (e.g., kg/m^3), and B_{vaw} represents the air-to-leaf bioconcentration factor on a fresh (i.e., wet) plant mass basis. If benzene is assumed to exist in air entirely as a vapor, then F_v equals 1. It has been suggested that B_{vaw} can be correlated with the chemical's water-air and octanol-water partition coefficients.

Table 4-9 presents root uptake and air-to-leaf bioconcentration factors for benzene. Experimentally determined root uptake bioconcentration for benzene in barley plants range from 2 to 17 and in cress plants from 1.9 to 10. Although B_{vaw} has not been measured for benzene, there are a number of the air-water bioconcentration correlation that have been proposed in the literature

$$\log B_{vaw} = 1.25 \log H_i + 4.06 \quad (\text{Calamari et al., 1987}) \quad (4-19)$$

$$\log B_{vaw} = -1.95 + 1.14 \log K_{ow} - \log H_i' \quad (\text{Bacci et al., 1990a}) \quad (4-20)$$

$$B_{vaw} = 0.19 + 0.7/H_i' + 0.05 K_{ow}/H_i' \quad (\text{Paterson et al., 1991}) \quad (4-21)$$

$$B_{vaw} = 0.022 K_{ow}/H_i' \quad (\text{Bacci et al., 1990b}) \quad (4-22)$$

Table 4-9. Root Uptake and Air-to-Leaf Bioconcentration Factors for Benzene*

BCF Type	Bioconcentration (dimensionless)	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
Root uptake ^(a)	2.0	dimensionless	NR	NR	Measured ^(b)	Hattemer-Frey and Travis, 1990	Scheunert et al., 1985
Root uptake ^(a)	17 ^(c)	dimensionless	NR	281-298	Measured	Topp et al., 1989	
Root uptake ^(a)	2.3 ^(c)	dimensionless	NR	281-298	Measured	Topp et al., 1989	
Root uptake ^(a)	2.9 ^(c)	dimensionless	NR	281-298	Measured	Topp et al., 1989	
Root uptake ^(a)	4.6 ^(c)	dimensionless	NR	281-298	Measured	Topp et al., 1989	
Root uptake ^(a)	10 ^(d)	dimensionless	NR	281-298	Measured	Topp et al., 1989	
Root uptake ^(a)	2.3 ^(d)	dimensionless	NR	281-298	Measured	Topp et al., 1989	
Root uptake ^(a)	1.9 ^(d)	dimensionless	NR	281-298	Measured	Topp et al., 1989	
Air-to-leaf ^(e)	0.12 ^(e)	dimensionless	NR	NR	Calculated ^(e)	Hattemer-Frey and Travis, 1990	
Air-to-leaf	17 ^(f)	dimensionless	NR	NR	Calculated	Section 4.2.4	Calamari et al., 1987
Air-to-leaf	0.66 ^(g)	dimensionless	NR	NR	Calculated	Section 4.2.4	Bacci et al., 1990

Table 4-9. Root Uptake and Air-to-Leaf Bioconcentration Factors for Benzene*
(Continued)

BCF Type	Bioconcentration (dimensionless)	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
Air-to-leaf	34 ^(b)	dimensionless	NR	NR	Calculated	Section 4.2.4	Paterson et al., 1991
Air-to-leaf	1.2 ^(b)	dimensionless	NR	NR	Calculated	Section 4.2.4	Bacci et al., 1990

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) Root uptake bioconcentration factor defined as (Topp et al., 1989): $B_v = \frac{\text{concentration of C in dry plant matter (as benzene)}}{\text{concentration of C in dry soil}}$

(b) Value reported as "soil-to-root bioconcentration factor": $B_v = \frac{C_r}{C_s}$

C_r = 0.01 accumulated benzene in cress and barley
 C_s = 0.005 ppm concentration of benzene in soil

(c) Time of exposure: 12, 33, 71, 125 days - BARLEY PLANTS.

(d) Time of exposure: 12, 33, 79 days - CRESS PLANTS. Composition of soil 2.06% of org. C; pH = 6.4.

(e) Air-to-leaf bioconcentration factor (Hattermer-Frey and Travis, 1990). $B_{va} = 5.0 \times 10^{-6} K_{ow}/H$

(f) Calculated using equation $\log B_{vsw} = 1.25 \log H_i + 4.06$ (see Eq. 4-20 in the text).

(g) Calculated using equation $\log B_{vsw} = -1.95 + 1.14 \log K_{ow} + \log H_i'$ (see Eq. 4-21 in the text).

(h) Calculated using equation $B_{vsw} = 0.19 + 0.7/H_i' + 0.05 K_{ow}/H_i'$ (see Eq. 4-22 in the text).

(i) Calculated using equation $B_{vsw} = 0.022 K_{ow}/H_i'$ (see Eq. 4-23 in the text).

where B_{vw} is based on wet mass, and K_{ow} and H_i' are the dimensionless octanol/water constants and Henry's Law constant as previously defined. It is noted that B_{vs} is related to B_{vw} .

$$B_{vw} = B_{vs} \times f_{dw} \quad (4-23)$$

Using, for example, a $\log K_{ow}$ of 2.13, an H_i value of $5.5 \times 10^{-3} \text{ atm} \cdot \text{m}^3/\text{mol}$ and an H_i' value of 0.22, a range of 0.66 - 34 was obtained for B_{vw} from Eqs. 4-19 - 4-22. It must be noted that benzene was not used as a study chemical in the development of the above correlations. Thus, the above estimates of B_{vw} values for benzene should only be regarded as estimates of the order of magnitude of B_{vw} for benzene.

4.2.5 Biotransfer Factors for Benzene in Milk, Beef, and Eggs

The concept of biotransfer factor (B_{TF}) addresses partitioning through food uptake. It has been suggested in the literature that the biotransfer factor (B_{TF}) may be more useful than BCFs in addressing exposure via food uptake since chemical exposure to feedstock animals may occur through both food and water pathways (Travis and Arms, 1988).

At steady state, the pathway specific biotransfer factor, B_{TF_i} , for pathway i , can be expressed as

$$B_{TF_i} = C_j / L_i C_{in} \quad (4-24)$$

and the overall biotransfer factor, B_{TF} , can be expressed as (Cohen, 1989)

$$B_{TF} = \frac{C_j}{\sum_{i=1}^N L_i C_{in}} = \left[\sum_{k=1}^N E x_k H_{kj} + K_j V_j \right]^{-1} \quad (4-25)$$

V_j is the volume of the receptor and C_j and C_m are the concentrations of the contaminant in the receptor (or target organ) and the media associated with the receptor route and N is the total number of intake pathways. L_i represents the intake rate and Ex_k is the outflow stream associated with the particular pathway. H_{kj} is the partition coefficient between receptor j and outflow stream k . The overall biochemical transformation of a given contaminant via first order reaction kinetics is given by the rate constant K_j while the subscript k represents a specific elimination pathway. For example, one can define a B_{TF} for the concentration of a contaminant in cow's milk where $\sum_{i=1}^N L_i C_m$ is the total contaminant intake during grazing, water drinking, and inhalation. In general, the B_{TF} is not constant since V_j , the volume of the receptor, may vary with time, and the partition coefficient, H_{kj} , and the reaction rate constant, K_j , are likely to be functions of the activity of the receptor. Thus, one is led to conclude that B_{TF} and B_{TFi} are likely to be time variant parameters. Despite this above concern, the concept of biotransfer factors is rooted in environmental exposure assessment.

As previously noted, feedstock animals are exposed to benzene through ingestion of contaminated feed crops and drinking water, as well as direct inhalation. Human exposure can subsequently result from ingestion of contaminated animal products. Assessing the magnitude of human exposure to a contaminant such as benzene from ingestion of animal products depends largely on the ability to predict the extent of its bioaccumulation in aquatic and terrestrial food chains. Biotransfer factors for organics in beef and milk have been found to correlate with the equilibrium octanol/water partition coefficient directly proportional to K_{ow} (Travis and Arms, 1988), although the concept of B_{TF} should be regarded as a transport parameter rather than simply a physicochemical property (Cohen, 1989).

The biotransfer factors for milk (B_m) and meat (beef; B_b) have been defined by Travis and Arms (1988) as follows:

$$B_m = \frac{(\text{concentration in milk (mg/kg)})}{(\text{daily intake of organic (mg/d)})} \quad (4-26)$$

$$B_b = \frac{(\text{concentration in meat (mg/kg)})}{(\text{daily intake of organic (mg/d)})} \quad (4-27)$$

where measured concentration of organics in milk or meat fat are converted on a whole milk or fresh meat basis, assuming meat is 25% fat and whole milk is 3.68% fat.

As summarized in Table 4-10, Travis and Arms (1988) derived a $\log K_{ow}$ vs. $\log B_m$ correlation based on data for 28 organic chemicals in milk (benzene was not included) which yielded the following equation:

$$\log B_m = -8.10 + \log K_{ow} \quad 2.81 < \log K_{ow} < 6.89 \quad (4-28)$$

In the above equation, for which the regression correlation coefficient was 0.74, B_m was based on data for ingestion only and did not include contaminant uptake via inhalation or dermal absorption. Using Eq. 4-28 and a $\log K_{ow}$ value of 2.13 (Fujita et al., 1964), $\log B_m$ equals -5.97 (or $B_m = 1.07 \times 10^{-6}$) which implies very little transfer of benzene to milk due to ingestion.

The validity of applying the regression equations of Travis and Arms (1988) may be questionable since benzene was not one of the chemicals used for the regression analysis and its $\log K_{ow}$ value of 2.13 is below the range of $\log K_{ow}$ from which the correlation was derived. One is cautioned that in applying K_{ow} correlations derived from regression analysis, it is important to verify that the value of K_{ow} is within the range of applicability of the correlation. It is important to note that B_{TF} correlations determined by Travis and Arms (1988) are subject to uncertainties in the input data from which B_{TF} s were derived. For instance, McKone and Ryan (1989) noted that the uncertainty in the Travis and Arms (1988) correlations for 95% confidence interval for both the feed to milk biotransfer factor, B_m , and the feed to meat biotransfer factor, B_b , is approximately 2 orders of magnitude.

Table 4-10. Feed to Milk Transfer Factor (B_m)^(a) for Benzene*

Feed-to-Milk Transfer Factor	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
1.07×10^{-6}	d/kg	NR	NR	Calculated ^(b)	Hattemer-Frey and Travis, 1990	Travis and Arms, 1988

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) The feed to milk conversion factor (B_m) is a biotransfer factor (BTF) that is defined as (Travis and Arms, 1988):

$$B_m = \frac{\text{concentration in milk (mg/kg)}}{\text{daily intake of organic (mg/d)}}$$

(b) Based on octanol/water partition coefficient (K_{ow}) using the following equation:

$$B_m = -8.10 + \log K_{ow}$$

where $\log K_{ow} = 2.13$.

A log B_b vs. log K_{ow} correlation was proposed by Travis and Arms (1988) as given below

$$\log B_b = -7.6 + \log K_{ow} \quad (4-29)$$

for which the regression correlation coefficient was reported as 0.81. Using the value for log K_{ow} for benzene (2.13), log B_b equals -5.47 (see Table 4-11).

Experimentally determined or calculated biotransfer factor values for feed to egg were not found in the literature. The CAPCOA guidelines, for example, assume that the biotransfer for eggs is the same as that of meat, this appears to be a reasonable approximation in the absence of data to the contrary.

The measurement-specific definition of BCF and B_{TF} above must be distinguished from other terms used to describe the increase in chemical concentration in an organism via the food chain. Such terms include biomagnification and bioaccumulation (Lyman et al., 1990). Biomagnification refers to a further increase in concentration attributable to uptake from food. Bioaccumulation is a broader term that indicates uptake from all sources and thus includes effects of both biomagnification and bioconcentration (Clark et al., 1988). These terms are associated with increasing concentrations along a food chain, which could result in higher concentrations factors in top-order consumers.

The overall bioaccumulation factor K_b can be shown to be related to the biotransfer factors by the following relation (Cohen, 1989):

$$K_b = C_j/C_i = B_{TF} \left(\sum_{i=1}^N L_i C_m \right) / C_i \quad (4-30)$$

where C_j is the concentration of the contaminant in the receptor, C_i is the concentration in the media most directly associated with the exposure route, B_{TF} is the biotransfer factor, L_i is the intake rate via food intake, water drinking, and inhalation, and C_m is the concentration in either the food (e.g., pasture grass), drinking water, or inhaled air.

Bioaccumulation factors are a function of the receptor type, the chemical type, and temperature. The bioaccumulation factor is equivalent to the bioconcentration factor when the exposure takes place primarily via contact with a single medium (e.g., inhalation of a volatile chemical such as benzene). The above approach assumes implicitly that K_b is time invariant. For biota, K_b (or BCF) is often correlated with K_{ow} (Kenaga and Goring, 1980; Mackay, 1982; Veith and Rosian, 1983).

4.2.6 Bioconcentration in Beef

The accumulation of contaminants in cattle beef due to dietary intake can also be estimated from the bioconcentration factor for beef defined as:

$$BCF_m = \frac{\text{concentration in beef}}{\text{concentration in diet}} \quad (4-31)$$

A set of correlations for BCF_m were proposed by Kenaga (1980b) as given below:

$$\log BCF_m = -0.495 (\log S) - 1.476 \quad (4-32a)$$

$$\log BCF_m = 0.5 (\log K_{ow}) - 3.457 \quad (4-32a)$$

where S is the aqueous solubility (mole fraction) and K_{ow} and K_{oc} are as defined previously. The regression correlation coefficients for Eq. 4-32 range from 0.79 to 0.82.

4.2.7 Bioavailability and Pharmacokinetics of Benzene

The bioavailability of a chemical is defined as the fraction of a compound in a matrix that is released from that matrix, absorbed by an organism, and hence, is available to elicit a biological effect. The release and uptake of a chemical constitute facets of bioavailability, although its biological effect is often used as a measure of bioavailability. Since risk is considered to be a function of both exposure and toxicity, bioavailability is an important consideration in determining potential risk from airborne contaminants (SCAQMD, 1988).

Table 4-11. Feed to Meat Transfer (B_b)^(a) Factor for Benzene*

Feed-to-Meat Transfer Factor	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
2.9×10^{-6}	d/kg	NR	NR	Calculated ^(b)	Hattemer-Frey and Travis, 1990	Travis and Arms, 1988

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) The feed to meat (beef) conversion factor (B_b) is a biotransfer factor defined as (Travis and Arms):

$$B_b = \frac{\text{concentration in meat (mg/kg)}}{\text{daily intake of organic (mg/d)}}$$

(b) Based on octanol/water partition coefficient (K_{ow}) using the following equation:

$$\log B_b = -7.735 + 1.033 \log K_{ow}$$

where $\log K_{ow} = 2.13$. Note that this correlation is slightly different than Eq. 4-29. From Eq. 4-29 $\log B_b = -5.47$ while the above correlation yields $\log B_b = -5.53$.

Bioavailability is often considered when assessing dose from inhalation and ingestion pathways. For ingestion routes, CAPCOA (1992) allows for using compound-specific bioavailability factors where evidence warrants but does not provide any values for benzene. The CAPCOA (1992) guidelines assume 100% absorption for inhaled compounds. Since benzene is likely to be present primarily in the gaseous phase, the assumption of 100% bioavailability is considered reasonable. Once absorbed through the lung, pharmacokinetic studies have identified only two routes of elimination, either exhalation or metabolism in the liver, and to a lesser extent metabolism in the bone marrow. Although the exact mechanism of toxicity is unknown, it is generally accepted that benzene must be metabolized before its toxic effects are apparent (Sammatt et al., 1979; Sawahata et al., 1985; Gad El-Karim et al., 1986; Kalf, 1987; Gaido and Wierda, 1987 as cited in Travis et al., 1990; Medinsky et al., 1989). Moreover, studies with toxicokinetic models have suggested that only a fraction of the benzene inhaled by the human receptor is metabolized in the body (Travis et al., 1990; Hattemer-Frey and Travis, 1990).

4.3 Intermedia Transport Parameters

The following subsections define the specific intermedia transport factors considered for this study as well as the results of the corresponding literature review.

4.3.1 Diffusion Coefficients of Benzene in Air and Water

Molecular diffusion is the net transport of a molecule within a single phase (e.g., liquid or gas) that results from intermolecular collisions rather than turbulence or bulk transport. Diffusion can result from pressure, temperature, and concentration gradients but under environmental conditions, only diffusion due to concentration gradient is considered. The diffusive flux due to concentration gradients is defined by Fick's Law as:

$$J_A = -D_{AB} dC_A/dx \quad (4-34a)$$

in which J_A is the diffusion flux for compound A (e.g., mg/m²s), dC_A/dx is the concentration gradient along the x direction and D_{AB} is the diffusion coefficient of A in medium B (e.g., units of cm²/s). For example, for air/water exchange processes, molecular diffusion dominates chemical transport near the air/water interphase (in both the air and water phases). In general, the mass flux, N , across an interface is expressed by an equation of the form

$$N = K \Delta C \quad (4-34b)$$

in which K is a mass transfer coefficient and ΔC is a concentration driving force. Correlations of mass transfer coefficients include a dependence on the molecular diffusivity which can be estimated as described below.

Table 4-12 presents values for diffusion coefficients of benzene in air and water. The experimental diffusion coefficients in air and water are 0.096 cm²/s at 298.2 K and 1.02×10^{-5} cm²/s at 298 K, respectively (Cussler, 1984). Diffusion coefficients in air can be calculated by using the correlation of Fuller et al. (1966)

$$D_{BA} = \frac{10^{-3} T^{1.75} \sqrt{M_T}}{P (V_A^{1/3} + V_B^{1/3})^2}, \text{ cm}^2/\text{s}, \text{ where } M_T = \frac{M_A + M_B}{M_A M_B} \quad (4-35)$$

in which the subscripts A and B refer to air and benzene, respectively, T is the temperature (K), M is the molecular weight, P is the pressure (atm), and V_A and V_B are the molar volumes (cm³/mol) for air and the gas in question, respectively.

Correlations commonly used to calculate diffusion coefficients in water are given below.

Wilke and Chang (1955):

$$D_{BW} = \frac{7.4 \times 10^{-8} (\phi_w M_w)^{1/2} T}{\eta_w V_B^{0.6}}, \text{ cm}^2/\text{s} \quad (4-36)$$

Table 4-12. Diffusion Coefficient^(a) in Air and Water for Benzene*

Media	Diffusion Coefficient (cm ² /s)	Reported Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
Air	0.096	0.096	cm ² /s	NR	298.2	Measured	Cussler, 1984	
Air	0.087	0.087	cm ² /s	NR	293	Calculated	Cohen and Ryan, 1989	Bird et al., 1960
Air	0.088	0.088	cm ² /s	NR	NR	Calculated ^(b)	Mackay and Yeun, 1983	Reid et al., 1977
Air	0.05 ^(c)	157	m ² /year	NR	NR	Calculated	McKone and Layton, 1986	Lyman, 1982
Air	0.088	0.088	cm ² /s	NR	298	NR	CARB and CDHS, 1984	Thibodeaux, 1979
Water	1.02×10 ⁻³	1.02×10 ⁻³	cm ² /s	NR	298	Measured	Cussler, 1984	
Water	1.02×10 ⁻³	10.2×10 ⁻⁶	cm ² /s	NR	293	Calculated ^(d)	Cohen and Ryan, 1989	Bird et al., 1960
Water	9.57×10 ⁻⁶	0.957×10 ⁻³	cm ² /s	NR	NR	Calculated ^(d)	Mackay and Yeun, 1983	Reid et al., 1977
Water	6×10 ^{-6(a)}	0.02	m ² /year	NR	NR	Calculated ^(d)	McKone and Layton, 1986	Lyman, 1982
Seawater	7.8×10 ⁻⁶	7.8×10 ⁻⁶	cm ² /s	NR	292	Calculated ^(d)	Wakeham, 1986	Wilke and Chang, 1955

Table 4-12. Diffusion Coefficient^(a) in Air and Water for Benzene*
(Continued)

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) Diffusion coefficient defined according to Fick's Law:

$$J_A = -D_{AB} \frac{dC_A}{dX}$$

where J_A - diffusion flux

$\frac{dC_A}{dX}$ - concentration gradient

D_{AB} - diffusion coefficient

$$(b) \quad D_{BA} = \frac{10^{-3} T^{1.75} \sqrt{M_r}}{P(V_A^{1/3} + V_B^{1/3})^2}, \quad \text{cm}^2/\text{s}, \quad \text{Method of Fuller, Schettler, and Giddings [Fuller et al., 1966]}$$

(all variables are defined in Section 4.3.3)

$$M_r = \frac{M_A + M_B}{M_A M_B}$$

$$(c) \quad \text{Conversion from reported value:} \quad 157 \text{ m}^2/\text{year} \times \frac{(100 \text{ cm})^2}{\text{m}^2} \times \frac{1 \text{ year}}{3.15 \times 10^7 \text{ sec}} = 0.05 \text{ cm}^2/\text{sec}$$

$$(d) \quad D_{BW} = \frac{7.4 \times 10^{-8} (\phi_w M_w)^{1/2} T}{\eta_w V_B^{0.6}}, \quad \text{cm}^2/\text{s}, \quad \text{Wilke-Chang est. method [Wilke and Chang, 1955]}$$

(all variables are defined in Section 4.3.3)

where M_w is the molecular weight of water (g/mol), T is the temperature (K), η_w is the viscosity of water (cP), V_B is the molar volume of solute B at its normal boiling temperature (cm^3/mol), and ϕ_w is the solvent association factor which equals 2.6 for water (Wilke and Chang, 1955). Using Eq. 4-36 to calculate the diffusion coefficient of benzene in seawater, a value of $7.8 \times 10^{-6} \text{ cm}^2/\text{s}$ was obtained (Wakeham et al., 1986).

Hayduk and Laudie (1974):

$$D_{BW} = \frac{13.26 \times 10^{-5}}{\eta_w^{1.14} V_B^{0.589}} \quad , \quad \text{cm}^2/\text{s} \quad (4-37)$$

where η_w is the viscosity of water (cP) and V_B is the molar volume (cm^3/mol):

Hayduk et al. (1982):

$$D_{BW} = 1.25 \times 10^{-8} (V_B^{-0.19} - 0.292) T^{1.52} \eta_w^{\epsilon^*} \quad , \quad \text{cm}^2/\text{s} \quad (4-38)$$

where V_B is the molar volume (cm^3/mol) of solute, η_w is the viscosity of water (cP), and $\epsilon^* = (9.59/V_B) - 1.12$.

4.3.2 Gaseous Mass Transfer Across the Air-Water Interface

The traditional approach to calculating the flux of a compound between air and water phases is to use the two-film theory in which it is assumed that the concentrations immediately on either side of the interface are in equilibrium as can be expressed by a Henry's Law constant (Lewis and Whitman, 1924). The flux, N , can be expressed as:

$$N = K_G (C_g - H'C_l) = K_L (C_l - C_g/H') \quad (4-39)$$

where K_G and K_L are the overall mass transfer coefficients (cm/s) for the gas and liquid phase, respectively, H is a unitless Henry Law's constant, and C_g and C_l are concentrations

in gas and liquid phases, respectively. The overall mass transfer coefficients for the gas and liquid phase can be defined as:

$$1/K_G = 1/k_g + H'/k_l \quad (4-40)$$

$$1/K_L = 1/k_l + 1/H'k_g \quad (4-41)$$

where k_g is a gas-phase mass transfer exchange coefficient (cm/s) and k_l is a liquid-phase mass transfer coefficient. The important parameters that are needed in order to predict N are H' (see Section 4.2.1) and the mass transfer coefficients k_g and k_l . The mass coefficients depend on the prevailing turbulence level (as determined by water currents or wind), on temperature, on properties of the solute such as diffusivity, or molecular size (Mackay and Yeun, 1983), and on the depth of the water body (Cohen, 1986). Thus, one must ensure that k_g and k_l are determined for the appropriate environmental conditions. Predictive equations, appropriate for screening-level analysis, that can be used to estimate k_g and k_l are given in Sections 4.3.2.1 and 4.3.2.2.

Experimental studies of volatilization in laboratory wind-wave tanks have demonstrated that for most non-reactive and sparingly water soluble organics $H'k_g > k_l$; thus, for such chemicals, the liquid-side resistance to mass transfer is greater than the gas-side resistance. It is noted that benzene has a relatively high Henry's Law constant compared to most hydrophobic organic compounds (Lyman et al., 1990; Section 4.2.1) and abiotic degradation in the aqueous phase is not a significant loss process (Section 3.4). Thus, for benzene in an aqueous solution, k_l (Section 4.3.2.2), is the more important transport coefficient controlling benzene exchange between water and air. In general, for chemicals for which k_l is of the same order of magnitude as $H'k_g$, both k_l and k_g should be considered as given in Eqs. 4-39 - 4-41. In the case of evaporation of benzene from a pure benzene phase, however, the gas phase resistance dominates and k_g becomes the more important mass transfer coefficient to consider.

4.3.2.1 Air/Water - Air Side - Mass Transfer Coefficient (k_g) for Benzene

Numerous theories and empirical equations have been proposed to predict k_g . The theoretical expressions for k_g as proposed by Brutsaert (1975) are particularly useful for predicting k_g . For a rough surface, k_g is given by:

$$\frac{k_g}{U_{10}} = C_D^{1/2} \left[\epsilon_D^+ (C_D^{-1/2} - 5) + 7.3 Re_o^{0.25} Sc_a^{1/2} \right]^{-1}, \quad Re_o > 2 \quad (4-42)$$

and for a smooth surface, k_g is given by:

$$\frac{k_g}{U_{10}} = C_D^{1/2} \left[\epsilon_D^+ (C_D^{-1/2} - 13.5) + 13.6 Sc_a^{2/3} \right]^{-1}, \quad Re_o < 0.13 \quad (4-43)$$

in which the Schmidt number, Sc_a , is given by the ratio ν_a/D_a , where D_a is molecular diffusivity in air (Section 4.3.1), U_{10} is the wind speed at a reference height (usually 10 meters), C_D is the wind drag (or stress) coefficient, ϵ_D^+ is the ratio of the eddy momentum diffusivity (ϵ_m) to the eddy mass diffusivity (ϵ_D), often approximated to be near unity, and Re_o is the roughness Reynolds number. Eqs. 4-42 and 4-43 are strictly applicable to a neutral atmospheric condition. However, as suggested by Brutsaert (1975), Eqs. 4-42 and 4-43 are probably still satisfactory even under very unstable, but apparently not under stable conditions. For non-neutral conditions, the mass flux equations Eq. 4-39 must be used with caution since the bulk gas phase concentration as used in Eq. 4-39 may lie outside the dynamic sublayer (Brutsaert, 1975). Under such conditions, a detailed air quality model which considers the concentration profile at the air-side must be considered. Thus, one should regard the use of the estimation methods for k_g as given in this section as suitable for neutral conditions and for screening-level analysis for non-neutral conditions. The prediction of k_g for non-neutral conditions can be accomplished using the approach as presented by Brutsaert (1975). However, it should be noted that within the context of

screening-level analysis, as is the case in the CAPCOA model, the application of Eqs. 4-42 and 4-43 is sufficient especially for sparingly soluble hydrophobic organic compounds.

The use of Eqs. 4-42 and 4-43 requires the wind drag coefficient velocity as input. The wind-drag coefficient, C_D , is defined as (Wu, 1980)

$$C_D = \left(\frac{U_w^*}{U_{10}} \right)^2 \left(\frac{\rho_w}{\rho_a} \right) = \left(\frac{U_a^*}{U_{10}} \right)^2 \quad (4-44)$$

in which U_w^* is the surface shear velocity given by:

$$U_w^* = \sqrt{\frac{\tau_s}{\rho_w}} \quad (4-45)$$

where τ_s is the shear stress imparted by the wind on the water surface, ρ_w is the water density, ρ_a is the air density, and U_{10} is the wind speed measured at a reference height (usually 10m) above the water surface. It is noted that the water-side friction velocity U_w^* and U_a^* are related through the simple relation $\rho_a(U_a^*)^2 = \rho_w(U_w^*)^2$ which arises from the condition of stress equality at the air/water interface. Given wind speed profile data, one can estimate U_a^* using the following equation:

$$U_a^* = U_{10} k \left[\ln\left(\frac{z_{10}}{z_o}\right) - \psi_M\left(\frac{z}{L}\right) + \psi_M\left(\frac{z_o}{L}\right) \right]^{-1} \quad (4-46)$$

where k is the von Karman constant ($k = 0.4$), U_{10} is the velocity at the reference height, z_{10} , ψ_M is a stability function, and L is the Obukhov stability parameter (Holtslag and Van

Ulden, 1983; and reference therein). It is noted that for neutral conditions the function ψ_M is set to zero. The roughness Reynolds number, Re_o , is defined by:

$$Re_o = U_*^* z_o / \nu_a \quad (4-47)$$

where z_o is the effective surface roughness height and ν_a is the kinematic viscosity of air. The effective surface roughness height can be estimated for smooth water surfaces as (Brutsaert, 1975)

$$z_o = 0.135(\nu_a / U_*^*) \quad , \quad \text{cm} \quad (4-48a)$$

and for a rough surface,

$$z_o = a(U_*^*)^b \quad , \quad \text{cm} \quad (4-48b)$$

in which U_*^* is the air-side friction velocity (cm/s) and ν_a is the kinematic viscosity (cm/s²). The parameters a and b are given by $a = 1.69 \times 10^{-2}$ and $b = -1$ for $U_*^* \leq 6.89$ cm/s, and $a = 1.65 \times 10^{-4}$, $b = 1.4$ for $U_*^* > 6.89$ cm/s (Jirka and Brutsaert, 1984). An alternative correlation for z_o was proposed by Wu (1980) for a large water fetch in which z_o was expressed by:

$$z_o = 0.0144(U_*^*)^2 / g, \quad (g = 981, \text{ cm/s}^2) \quad (4-48c)$$

For a large water fetch, the wind-stress coefficient near neutral conditions can be estimated from (Cohen, 1983)

$$C_D = 8.5 \times 10^{-4} \quad , \quad U_{10} < 5 \text{ m/s} \quad (4-49a)$$

$$C_D = [0.85 + 0.11 (U_{10} - 5)] \times 10^{-3} \quad , \quad 5 \text{ m/s} \leq U_{10} \leq 20 \text{ m/s} \quad (4-49b)$$

$$C_D = 2.5 \times 10^{-3} \quad , \quad U_{10} > 20 \text{ m/s} \quad (4-49c)$$

or (Wu, 1980)

$$C_D = (0.8 + 0.065U_{10}) \times 10^{-3} \quad , \quad U_{10} \geq 1 \text{ m/s} \quad (4-50)$$

As an illustration of the above approach, the gas-side mass transfer coefficient as obtained from Eqs. 4-42, 4-43 (with linear interpolation in the region $0.13 \leq Re_o \leq 2$), and Eqs. 4-48b and 4-50 for z_o and C_D , respectively, for benzene at 20°C is given in Figure 4.1. Other alternate expressions for k_g under neutral (or near-neutral) conditions have been proposed in the literature. For example, Lyman (1990) recommends the correlation of Southworth (1979) for k_g

$$k_g = 1137.5 (V_{\text{wind}} + V_{\text{curr}}) \sqrt{\frac{18}{MW}} \quad , \quad \text{cm/hr} \quad (4-51)$$

where V_{wind} and V_{curr} are the velocities of the wind and water current, respectively (m/s), and MW is the molecular weight of the contaminant of interest. As an example, using $V_{\text{wind}} = 3 \text{ m/s}$ and $V_{\text{curr}} = 1 \text{ m/s}$, k_g for benzene is estimated as 2184 cm/hr. It is important to note that the atmospheric stability condition for which Eq. 4-51 applies was not reported. Moreover, the theoretical basis of the Southworth (1979) equation is questionable because of the linear additivity of the wind and air currents in Eq. 4-51. The hydrodynamic effects of the wind relative to the water current on the roughness and velocity of the water surface are likely to be very different, as supported by later researchers (cited by Cohen, 1986) who have found that the effect of wind velocity and current velocity on k_g vary by different powers. Finally, a convenient correlation for k_g , determined based on laboratory measurements in a small wind-wave tank (fetch < 3m) under near neutral conditions, was proposed by Mackay and Yeun (1983).

$$\frac{k_g}{U_*} = 46.2 \times 10^{-3} Sc_a^{-0.67} \quad (4-52)$$

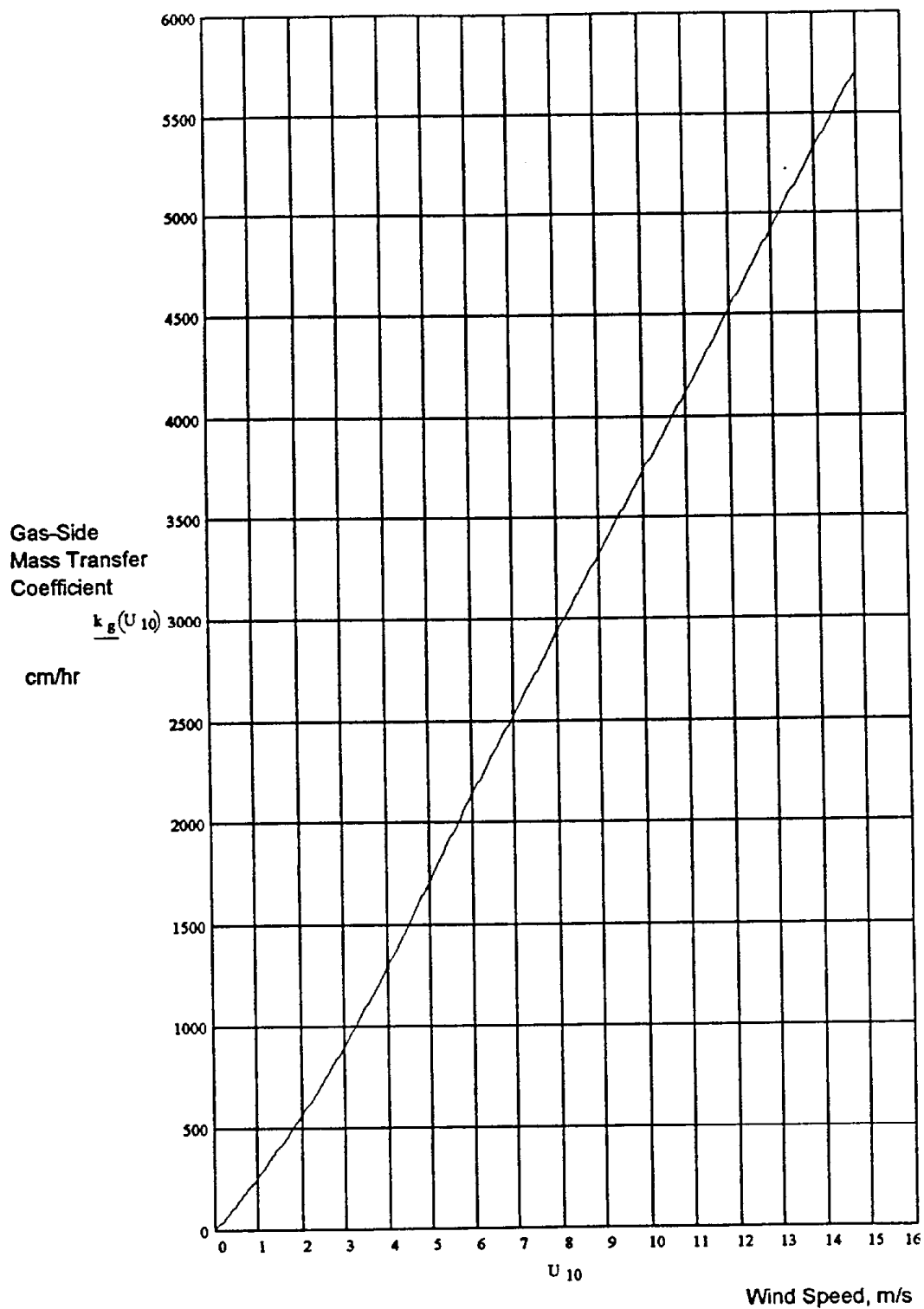


Figure 4.1. Gas-Side Mass Transfer Coefficient for Benzene at 20°C for Water/Air Mass Transfer at Large Fetch. (Based on the Correlation of Brutsaert, 1975).

Eq. 4-52 results in k_g values which are about 20%-40% higher than predicted by Eqs. 4-42 and 4-43. The higher prediction by the Mackay and Yeun (1983) correlation may be, in part, due to the difference in surface roughness condition in their short fetch wind-wave tank, for a given U_*^* , relative to the condition that would exist at long fetch.

4.3.2.2 Air/Water - Liquid Side - Mass Transfer Coefficient (k_l) for Benzene

The water-side mass transfer coefficient, k_l , for large water bodies (i.e., reservoirs, lakes, oceans) can be estimated using the theoretical correlation of Cohen and Ryan (1985), which was found to be in excellent agreement with available data for a water-side friction velocity in the range of 0.5-6 cm/s,

$$k_l/U_*^* = a Sc_w^{-n} \quad (4-53a)$$

in which Sc_w is the Schmidt number given by the ratio ν_w/D_w where ν_w is the water kinematic viscosity and D_w is the chemical molecular mass diffusivity in water. The constants a and n are weak functions of the dimensionless water surface velocity U_*^+ ($U_*^+ = U_s/U_*^*$, in which U_s is the wind-induced surface water velocity), given by:

$$\begin{aligned} a &= a_0 - a_1 \ln U_*^+ \\ n &= n_0 - n_1 \ln U_*^+ \end{aligned} \quad (4-53b)$$

where

$$\begin{aligned} a_0 &= 0.09691; a_1 = 0.01053; \\ n_0 &= 0.5778; n_1 = 0.01771 \end{aligned} \quad (4-53c)$$

For a long fetch (say $\geq 30m$), the surface velocity is equal to about 3.5% of the wind speed (i.e., $U_s = 0.035 U_{10}$), while for short fetch (say less than about 10m), $U_s \approx 0.020 U_{10}$ (Wu, 1975; Plate and Friedrich, 1984). Eq. 4-53a was found to be in excellent agreement with laboratory data from wind-wave facilities with an average error of about 16 percent. As an illustration, the dependence of k_l on wind speed for benzene at 20°C is shown in Figure 4.2 where Eqs. 4-45 and 4-50 were used to determine U_*^* .

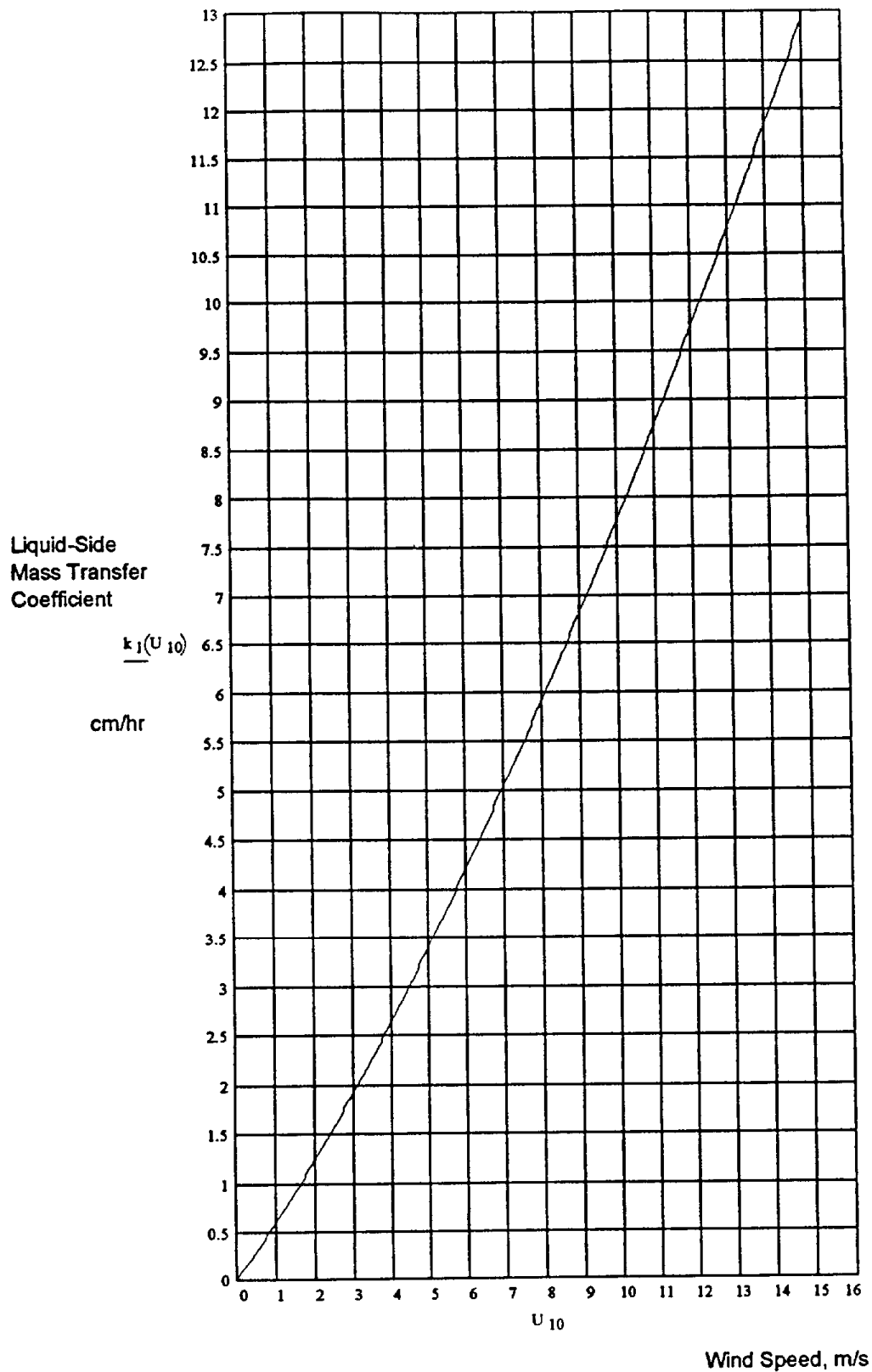


Figure 4.2 Liquid-Side Mass Transfer Coefficient for Benzene for Water/Air Mass Transfer at Large Fetch. (Based on the Theoretical Correlation of Cohen and Ryan, 1985).

The prediction of k_1 in flowing water bodies (e.g., rivers) requires consideration of the river current and the river depth (Cohen, 1986). There are numerous studies on the reaeration coefficient in flowing streams (O'Connor, 1983), and the water-side mass transfer coefficient k_1 can be estimated from the reaeration coefficient, k_r (e.g., hr^{-1}), by using the following relation:

$$k_1 = \left(\frac{D}{D_o} \right)^{1/2} h k_r \quad (4-54)$$

in which h is the depth of the water body (e.g., m), D is the mass diffusivity of the compound of interest (e.g., benzene), D_o is the mass diffusivity of oxygen at the temperature at which k_r was determined, and h is the river depth (Cohen, 1986). Lyman et al. (1982) recommended the following empirical correlations, which are based on field data, for predicting k_r :

$$k_r = 1.08 (1 + 0.17 F^2) (V_{\text{curr}} S)^{0.375}, \text{ hr}^{-1} \quad (4-55a)$$

$$k_r = 0.00102 V_{\text{curr}}^{2.695} h^{-3.085} S^{-0.823}, \text{ hr}^{-1} \quad (4-55b)$$

$$k_r = 638 V_{\text{curr}} S, \text{ hr}^{-1} \quad (4-55c)$$

in which S is the river bed slope (m drop/ m run), F is the Froude number ($F = V_{\text{curr}}/\text{gh}$), and h is the river depth (m). The use of an average value of k_r determined from the above three equations was recommended by Lyman et al. (1982). Other relations for k_r that are suitable when bed slope information is not available were recommended by Shen (1982), Lyman et al. (1990), and Shen et al. (1993). For example, the empirical correlation which was recommended by Shen (1982) and Shen et al. (1993) can be written as

$$k_r = 22.05 (1.024)^{T-20} U_s^{0.67} h^{-1.85}, \text{ hr}^{-1} \quad (4-55d)$$

in which T is the temperature ($^{\circ}\text{C}$), U_s is the water current (m/s), and h is the water depth (m). As an illustration, the liquid-side mass transfer coefficient, k_1 , obtained from Eqs. 4-54 and 4-55d for benzene at 20°C is shown in Figure 4.3.

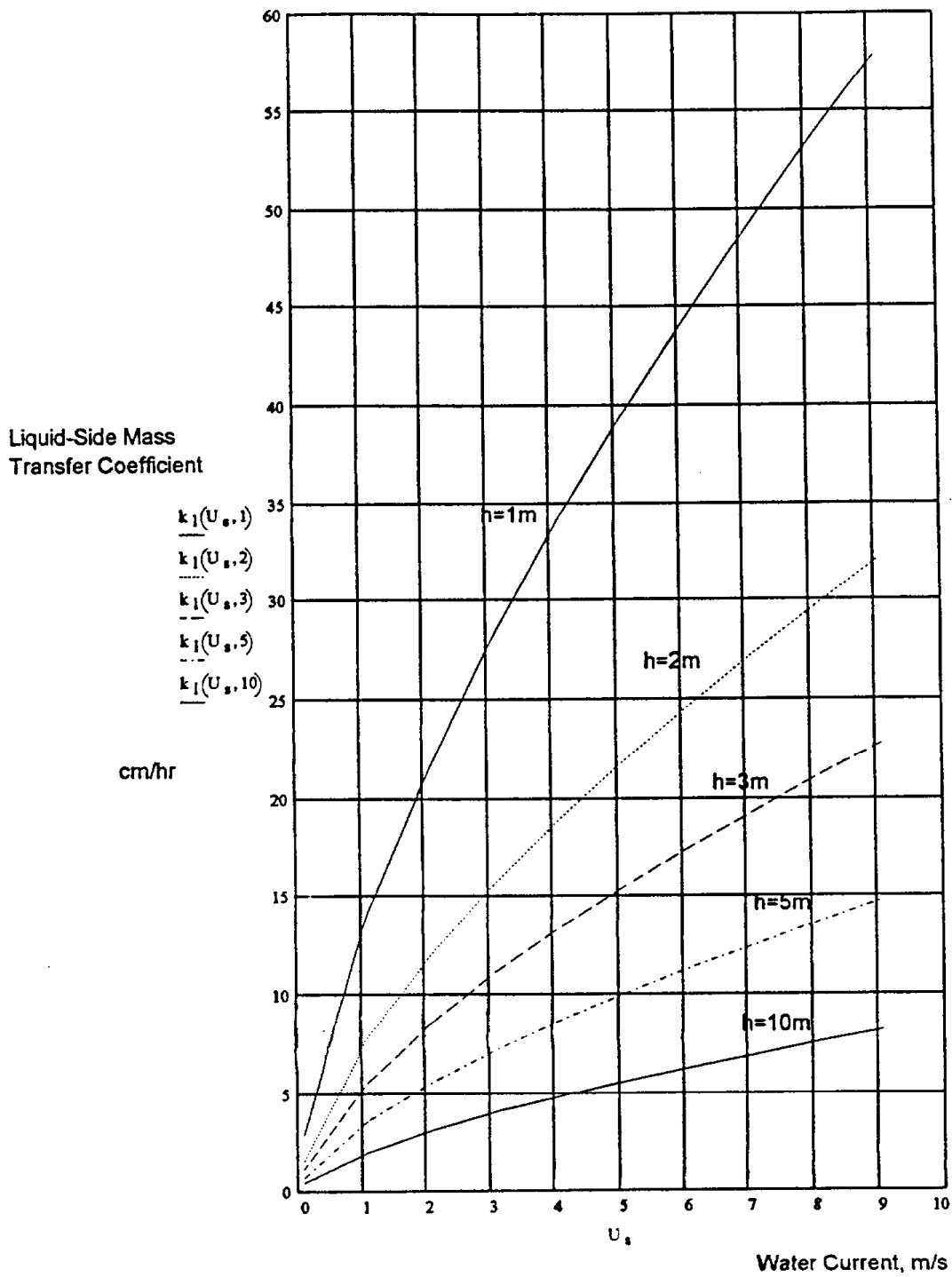


Figure 4.3. Liquid-Side Mass Transfer Coefficient for Benzene at 20°C for a Flowing River Based on Eq. 4-54 and 4-55d (h =river depth).

Example:

In order to estimate K_L for benzene for a neutral atmospheric condition, proceed along the following steps:

- 1) Select temperature, wind speed, and the correlation appropriate for the water body of interest.
- 2) Select a value of the Henry's Law constant from Table 4-5 and convert to dimensionless Henry's Law constant as per footnote (h) in Table 4-5.
- 3) Determine the value of k_l from a suitable correlation selected from Section 4.3.2.2 once a wind speed and type of water body are selected.
- 4) Determine k_g from either Eq. 4-42 or 4-43 depending on the resulting value for Re_o . Note that a value for U^* is required and this can be estimated from Eqs. 4-45, 4-49a - 4-49c, and 4-50 or from wind speed profile data.
- 5) Use Eq. 4-41 to determine K_L .

As an illustration, consider the volatilization of benzene from a large water body (i.e., large reservoir or lake) at 20°C. The diffusion coefficients in air and water were calculated to be 0.087 cm²/s and 8.96 × 10⁻⁵ cm²/s, respectively, using Eqs. 4-35 and 4-37. The kinematic viscosities for the air and water phases at 20°C were taken to be 0.15 cm²/s and 0.01 cm²/s, respectively (Reid et al., 1987). The gas-side mass transfer coefficient k_g at 20°C, obtained from Eqs. 4-42 and 4-43 (with linear interpolation of k_g in the region 0.13 ≤ Re_o ≤ 2), and Eqs. 4-48b and 4-50 for z_o and C_D , respectively, is given, as a function of wind speed, in Figure 4.1. The liquid-side mass transfer coefficient, k_l , obtained from Eq. 4-52, at 20° C, is given in Figure 4.2. As an example, at $U_{10} = 5$ m/s, $k_g = 1717$ cm/hr (Figure 4.1) and $k_l = 3.39$ cm/hr (Figure 4.2). Thus, using a value of 0.22 for the dimensionless Henry's Law constant (Table 4-5) leads to

$$K_L = \left[\frac{1}{3.39} + \frac{1}{0.22 \times 1714} \right]^{-1} = 3.36 \quad , \quad \text{cm/hr} \quad (4-55e)$$

Alternatively, one can directly determine K_L for benzene for the selected wind speed, using Figure 4.4. As can be seen from this example, the first term on the right hand side of Eq. 4-55e dominates. Thus, the liquid-side resistance ($1/k_l$) to benzene mass transfer across the water/air interface makes up about 99.1% of the total resistance ($1/K_L$) to mass transfer. Therefore, for benzene $K_L \approx k_l$, and since $Hk_g \gg k_l$ for all wind speeds, the approximation that $K_L = k_l$ is appropriate for benzene.

4.3.3 Dry Deposition Velocity for Benzene

The dry deposition flux of a gaseous chemical can be expressed by

$$N_A = V_d C_a \quad (4-56)$$

in which C_a is the mass of the pollutant in the particle phase per unit volume of air, and V_d is the overall chemical dry deposition velocity which can vary with wind speed and temperature. It is interesting to note that Sehmel (1980), in his critical review of particle and dry gas deposition velocity as it relates its use in atmospheric transport modes, observed that a deposition velocity of 1 cm/s is generally assumed, often due to the lack of a better estimate. The CAPCOA model currently uses deposition velocities of 2 cm/s and 5 cm/s for controlled and uncontrolled sources, respectively (see Table 4-13).

Experimentally determined values for the dry deposition velocity of benzene were found in the literature. However, the simple estimation method adapted by Cohen et al. (1990) can be used. According to this method, the dry deposition velocity is proportional to $D^{2/3}$ (where D is the molecular diffusivity of the chemical in air). Thus, if the dry deposition velocity for a given reference chemical is known, the value for benzene can be estimated using the relation

$$V_{d_B} = V_{d_A} \left(\frac{D_B}{D_A} \right)^{2/3} \quad (4-57)$$

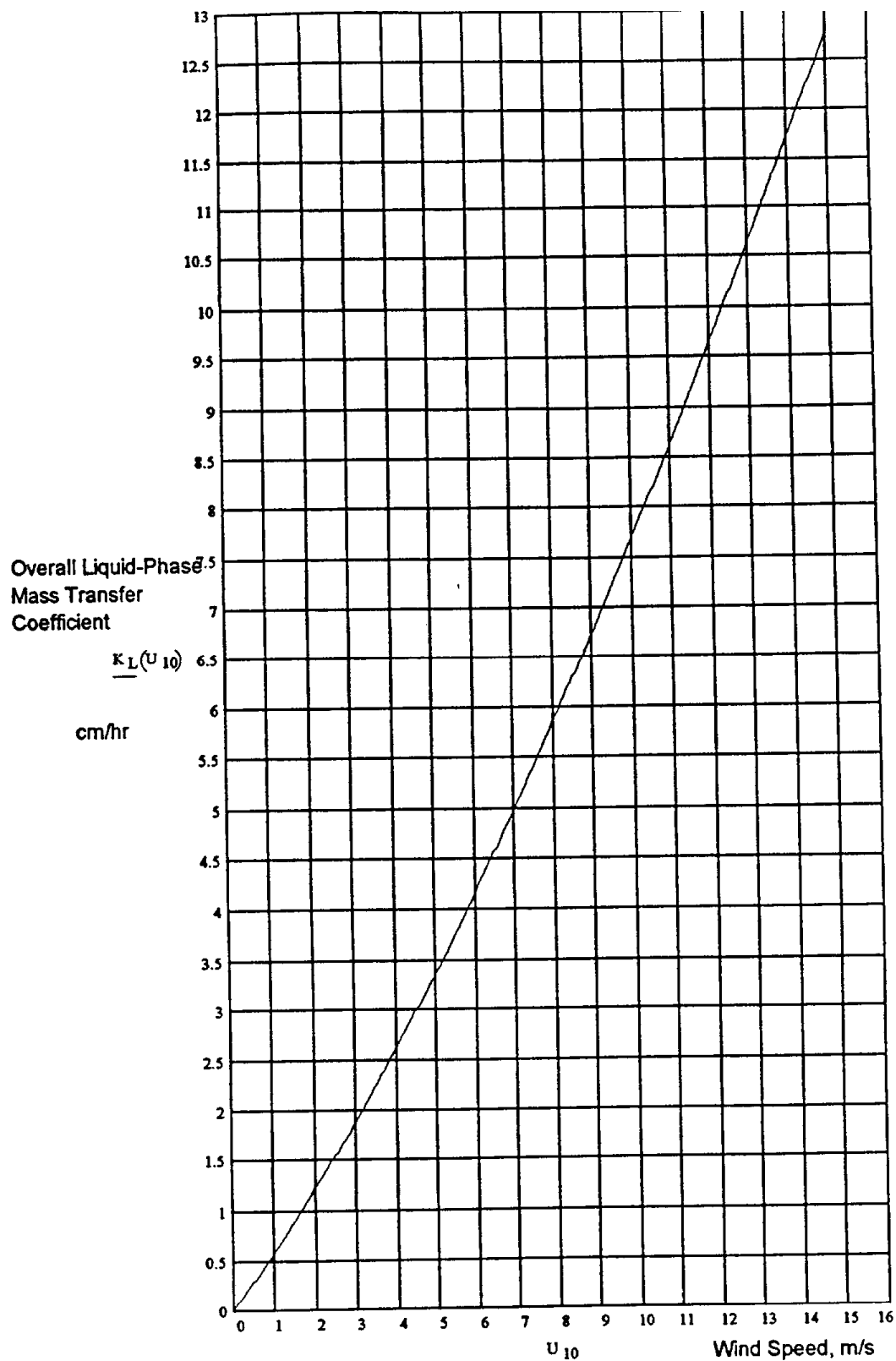


Figure 4.4 Overall Liquid-Side Mass Transfer Coefficient for Benzene for Water/Air Mass Transfer at Large Fetch. (Based on the Theoretical Correlations of Cohen and Ryan, 1985 and Brutsaert, 1975).

Table 4-13. Dry Deposition Velocity for Benzene* ^(a)

Dry Deposition Velocity (m/s)	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
0.02 ^(b)	NR	NR	Calculated	CAPCOA, 1991	NR
0.05 ^(c)	NR	NR	Calculated	CAPCOA, 1991	NR
2.8×10^{-4}			Calculated ^(d)	Section 4.3.3	
0.053			Calculated ^(e)	Section 4.3.3	

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

(a) Dry deposition velocity is known to be a function of wind speed and temperature (Davidson and Wu, 1989, and references therein.)

(b) Controlled source.

(c) Uncontrolled source.

(d) Eqs. 4-58 and 4-59 in Section 4.3.3 in this report.

(e) Eqs. 4-59 and 4-61 in Section 4.3.3 in this report.

where V_{dB} is the dry deposition velocity of benzene, V_{dA} is dry deposition velocity of a reference chemical for which deposition velocity is known (i.e., measured), at the meteorological and surface conditions of interest, D_B is a diffusion coefficient of benzene, and D_A is a diffusion coefficient of a reference chemical. The surface reactivity of the reference chemical should correspond, to the extent possible, to that of the chemical of interest.

Example: *Estimation of dry deposition velocity of benzene: [The deposition velocity for SO_2 and CO_2 was given by Sehmel (1980, 1984)].*

CO_2 as the reference chemical:

$$CO_2: V_{d_{CO_2}} = 0.3 \text{ cm/s}$$

$$D_{CO_2} = 0.155 \text{ cm}^2/\text{s at 298 K} \quad (\text{Reid et al., 1987})$$

(1) - Benzene

(2) - CO_2

$$V_{d_1} = V_{d_2} \left(\frac{D_1}{D_2} \right)^{2/3} \quad (4-58)$$

$$V_{d_1} = 0.3 \left(\frac{0.087}{0.155} \right)^{2/3} \quad (4-59)$$

$$V_{d_1} = 0.2 \text{ cm/s} \quad (4-60)$$

SO_2 as the reference chemical:

$$\text{air: } M_A = 28.97 \text{ g/mol (Lyman, 1990)}$$

$$SO_2: M_{SO_2} = 64 \text{ g/mol}$$

$$V_A = 20.1 \text{ cm}^3/\text{mol (Lyman, 1990)}$$

$$V_{SO_2} = 41.1 \text{ cm}^3/\text{mol (Fuller et al., 1966)}$$

From Eq. 4-35, at 25°C, the diffusion coefficient for SO₂ in air can be estimated as

$$D_{\text{SO}_2} = \frac{10^{-3} (298)^{1.75} \sqrt{0.05}}{1 [(20.1)^{1/3} + (41.1)^{1/3}]^2} = 0.121 \text{ cm}^2/\text{s} \quad (4-61)$$

(1) - Benzene

(2) - SO₂

$D_{\text{Benzene}} = 0.087 \text{ cm}^2/\text{s}$ at 298 K and 1 atm

$V_{d_{\text{SO}_2}} = 0.04 - 2.7 \text{ cm/s}$ for different deposition surfaces (0.04 cm/s was measured for asphalt and 2.7 cm/s was measured for an alfalfa surface)

$$V_{d_1} = V_{d_2} \left(\frac{D_1}{D_2} \right)^{2/3} \quad (4-62)$$

Lower Limit:

$$V_{d_1} = 0.04 \left(\frac{0.087}{0.121} \right)^{2/3} = 0.032 \text{ cm/s} \quad (4-63)$$

Upper Limit:

$$V_{d_1} = 2.7 \left(\frac{0.087}{0.121} \right)^{2/3} = 2.16 \text{ cm/s} \quad (4-64)$$

According to the above example, the dry deposition velocity for benzene is expected to be in the range of about 0.03 cm/s to 2.1 cm/s. Since SO₂ is reactive in the aqueous phase, a higher estimate would be obtained for the dry deposition velocity if the deposition surface for this reference gas (i.e., SO₂) was moist. Thus, the estimate of the dry deposition velocity based on CO₂ is more acceptable. Clearly, one has to ensure that the deposition surface for the reference chemical and for benzene are similar. Also, the dry deposition for benzene will depend on the prevailing meteorological and surface conditions in the area of interest.

Extensive data for deposition of various gases have been published and reviewed in the literature (Sehmel, 1980; Davidson and Wu, 1989).

4.3.4 Wet Deposition

Wet deposition (scavenging) can increase the overall deposition rate of benzene and thus, increase benzene concentration in the soil, water and vegetation due to direct deposition. Both rain and snow can remove benzene from air, however snowfall is not considered a significant removal process in most of the heavily populated regions in California. In addition, wet deposition is episodic; therefore, the climatological conditions of the location in question must be considered when evaluating the relative importance of wet deposition as a removal process.

The degree of wet deposition is usually estimated from knowledge of the washout ratio, W , defined as

$$W = C_{\text{rainwater}}/C_{\text{air}} \quad (4-65)$$

in which $C_{\text{rainwater}}$ and C_{air} are the concentrations (e.g., ng/m³) of benzene in rainwater (at ground level) and in the gaseous phase (i.e., in the atmosphere), respectively. Thus, the wet deposition flux, (e.g., ng/hr·m²), \dot{M}_w , is given by

$$\dot{M}_w = W \cdot R \cdot C_{\text{air}} \quad (4-66)$$

where R is the precipitation rate (e.g., m/hr). When compared with the washout ratios for highly water soluble, and hence efficiently removed, organic compounds of $W = 10^4$ - 10^5 (Eisenreich et al., 1981; Leuenberger et al., 1985; Atkinson, 1988), it appears that wet deposition of gaseous benzene will be of relatively minor importance as an atmospheric removal process for this compound.

Rain scavenging of benzene can be predicted using the detailed approach described by Lopez et al. (1989), Tsai et al. (1991), and Clay (1992). However, a simple upper-limit

estimate can be obtained by assuming that the raindrops are in equilibrium with the air phase when they reach ground level. This assumption is supported by the analysis of Cohen (1986) and Slinn (1978) who assert that raindrops falling through 10 meters of polluted atmosphere are nearly at equilibrium with gaseous chemical. Thus, the concentration of the dissolved chemical in rain, $C_w^{(d)}$ (e.g., ng/m³ water), is given by:

$$C_w^{(d)} = \frac{C_a^{(g)}}{H_{aw}} \quad (4-67)$$

in which $C_a^{(g)}$ is the concentration of the chemical in the atmosphere in the vapor phase (e.g., ng/m³ air), and H_{aw} is the dimensionless Henry's Law constant (i.e., $H_{aw} = C_a^{(g)}/C_w^{(d)}$).

4.4 Degradation

The following subsections define and review the specific degradation processes that were considered most applicable to benzene.

4.4.1 Reaction Half-life of Benzene in Air

The most significant atmospheric degradation process for benzene is its reaction with atmospheric hydroxyl (OH) radicals. Atkinson (1989) reviewed and critically evaluated the literature concerning the kinetics and mechanisms of the gas-phase reactions of benzene with the OH radical.

Based on a unit-weighted, least-squares analysis of the rate constants reported from several experimental techniques, including flash and laser photolysis-resonance fluorescence studies, the Arrhenius expression for reaction of benzene with OH radicals was reported by Atkinson (1989) over the temperature range 234-354 K. Based on this expression, the recommended value of the rate constant for reaction of benzene with OH radicals is 1.23×10^{-12} cm³/molec·s at 298 K, with an estimated overall uncertainty at 298 K of $\pm 30\%$ (Atkinson, 1989). This rate constant, and Arrhenius expression, is applicable for ~ 100 Torr

total pressure of argon diluent and is expected to be somewhat below the limiting high-pressure rate constant. At 298 K, the limiting high-pressure rate constant is expected to be $1.40 \times 10^{-12} \text{ cm}^3/\text{molec}\cdot\text{s}$ (Atkinson, 1989). Using this rate constant, an atmospheric lifetime² for benzene of 18 days was calculated for concentrations of OH of $1 \times 10^6 \text{ molec}/\text{cm}^3$ (Atkinson, 1988). The corresponding atmospheric half-life is 6.5 days and was calculated as $\tau_{1/2} = \ln 2 / (k_{\text{OH}} \times [\text{OH}])$.

While reaction of benzene with the OH radical is the dominant loss process during daylight hours, at night reaction with the gaseous nitrate (NO_3) radical must be considered. Atkinson et al. (1984) determined the rate constant at $296 \pm 2 \text{ K}$ for the gas phase reaction of NO_3 radicals with benzene using a relative rate technique. The rate constant obtained was $< 2.3 \times 10^{-17} \text{ cm}^3/\text{molec}\cdot\text{s}$ and this value was compared to other measured values of rate constants for benzene found in the literature of $< 3.5 \times 10^{-17} \text{ cm}^3/\text{molec}\cdot\text{s}$ (Japar and Niki, 1975) and $< 1.1 \times 10^{-17} \text{ cm}^3/\text{molec}\cdot\text{s}$ (Atkinson et al., 1984). Using a rate constant for the reaction of benzene with NO_3 radicals of $2.3 \times 10^{-17} \text{ cm}^3/\text{molec}\cdot\text{s}$, the calculated atmospheric half-life of benzene for concentrations of NO_3 of $2 \times 10^8 \text{ molec}/\text{cm}^3$ (Atkinson, 1988) is 4.7 years [$\tau_{1/2} = \ln 2 / (k_{\text{NO}_3} \times [\text{NO}_3])$].

Another potential degradation reaction is that of benzene with ozone (O_3). However, Pate et al. (1976) reported a rate constant for this reaction of $7 \times 10^{-23} \text{ cm}^3/\text{molec}\cdot\text{s}$, which for a typical atmospheric concentration of ozone of $7 \times 10^{11} \text{ molec}/\text{cm}^3$ (Singh et al., 1978) corresponds to an atmospheric half-life of 448 years [$\tau_{1/2} = \ln 2 / (k_{\text{O}_3} \times [\text{O}_3])$].

When compared to the calculated atmospheric lifetime against reaction with OH radicals, it is seen that reactions with ozone or NO_3 radicals are insignificant as gas phase atmospheric loss processes for benzene. Thus, reaction with OH radicals is the only important gas phase removal process for benzene. The reaction rate constants and their corresponding half-lives are summarized in Table 4-14.

² Atmospheric lifetime is defined as the time for the compound to decay to 37 % of its original concentration (Atkinson, Atmospheric Transformations of Automotive Emissions in Air Pollution, the Automobile, and Public Health, Watson et al.(eds.), 1988).

Table 4-14. Reaction Half-life of Benzene in Air*

Reaction Half-life ^(a) (days)	Reported Value	Reported Units	Reported Uncertainty	Temperature (K)	Technique	Reference	Source Cited
6.5 ^(b)	1.23×10^{-16}	cm ³ /molec-s	$\pm 30\%$	298	Reported as measured	Atkinson, 1989	
10 ^(b)	$0.8 \times 10^{-12(c)}$	cm ³ /molec-s	NR	300	Measured	U.S. PHS, 1989	Cox et al., 1980
10 ^(b)	$0.8 \times 10^{-12(c,d)}$	cm ³ /molec-s	(e)	NR	Measured	Cox et al., 1980	
24.5	24.5	days		NR	Measured	U.S. PHS, 1989	Cox et al., 1980
6.2 ^(b)	$1.3 \times 10^{-12(c)}$	cm ³ /molec-s	NR	NR	Calculated	Cox et al., 1980	Atkinson et al., 1979
6	6	days	NR	NR	NR	Hattemer-Frey and Travis, 1990	U.S. EPA, 1986a
6.2 ^(b)	$0.13 \times 10^{-11(c)}$	cm ³ /molec-s	NR	298	NR	U.S. PHS, 1989	Gaffrey and Levin, 1979
7.04 ^(b)	$0.114 \times 10^{-11(c)}$	cm ³ /molec-s	NR	298	NR	U.S. PHS, 1989	Lorenz and Zellner, 1983
4.7 years ^(e)	$< 2.3 \times 10^{-17(d)}$	cm ³ /molec-s	NR	296 ± 2	Measured	Atkinson et al., 1984	Atkinson et al., 1984
	$< 3.5 \times 10^{-17(d)}$	cm ³ /molec-s	NR	NR	Measured	Atkinson et al., 1984	Japar and Niki, 1975
4.48 years ⁽ⁱ⁾	$< 1.1 \times 10^{-17(d)}$	cm ³ /molec-s	NR	NR	Measured	Atkinson et al., 1984	Atkinson et al., 1984
	$7 \times 10^{-23(h)}$	cm ³ /molec-s	± 0.004	297 ± 2	Measured	Atkinson, 1988	Pate et al., 1976

NR = Not Reported.

* Listed order is by decreasing confidence in reported values (see Section 4.0).

Table 4-14. Reaction Half-life of Benzene in Air*
(Continued)

- (a) When not reported in days, the reaction half-life (τ) was calculated from the reaction rate constant (k) which is an Arrhenius expression based on temperature and pressure (see footnotes b and c below).
- (b) Conversion from reported value is from the equation: $\tau_{1/2} = \frac{\ln 2}{k_{OH} [OH]}$
- where k_{OH} is the OH radical rate constant and $[OH]$ is assumed to be 1×10^6 molec/cm³ (Atkinson, 1988). The calculated half-life ($\tau_{1/2}$) is in seconds, the conversion to days is accomplished by dividing by 86,400 s/day.
- (c) Rate constant for the reaction of benzene with OH radicals.
- (d) Absolute value based on value of 8×10^{12} cm³/molec-s for the reaction of OH with ethylene.
- (e) Uncertainty described by author as large due to slow decay of benzene.
- (f) Rate constant for the reaction of benzene with NO₃ radicals.
- (g) Half-life was calculated as follows: $\tau_{1/2} = \frac{\ln 2}{k_{NO_3} [NO_3]}$

where k_{NO_3} is the NO₃ radical rate constant and $[NO_3]$ was assumed to be 2×10^8 molec/cm³.

- (h) Rate constant for the reaction with O₃.

- (i) Half-life was calculated as follows: $\tau_{1/2} = \frac{\ln 2}{k_{O_3} [O_3]}$

where k_{O_3} is the O₃ rate constant and $[O_3]$ was assumed to be 7×10^{11} molec/cm³.

4.4.2 Biodegradation of Benzene in Water and Soil

Microbial degradation of benzene is influenced by many factors such as microbial population, benzene concentration, dissolved oxygen, the availability of nutrients, other sources of carbon, inhibitors, temperature, and pH. Unfortunately, in most cases, biodegradation constants are not directly reported in the literature. Thus, where biodegradation rate constants for benzene were not reported in research papers reviewed for this study, they were calculated, whenever feasible, based on information available in the papers. Biodegradation rate constants (k) were determined assuming first-order kinetics for biodegradation processes. The first-order rate law states that the rate is the product of the rate constant and the chemical (substrate) concentration (i.e., $dC/dt = -kC$). The following form of the first-order rate law equation was used to calculate biodegradation rate constants presented in Table 4-15

$$\ln \frac{C}{C_0} = -kt \quad (4-68)$$

where C_0 is initial benzene concentration, C is benzene concentration at time t , k is a rate constant, and t is a time interval. The assumption of first order kinetics is reasonable at low benzene concentrations, in homogeneous media, or as a first order approximation. The rate constants were subsequently used to calculate the biodegradation half-life ($\tau_{1/2}$) of benzene.

$$\tau_{1/2} = 0.693/k \quad (4-69)$$

From the results in Table 4-15, it can be seen that the fastest biodegradation rates for benzene were measured under aerobic conditions with nutritional enrichment. As expected, benzene biodegradation under anaerobic conditions is much slower than under aerobic conditions. It can also be seen that there is a wide range of values for biodegradation rate constants and corresponding biodegradation half-lives for benzene which can be attributed to different conditions for each experiment. Because experimental methods for measuring biodegradation rates are not standardized, the results are not comparable and apply only to a particular set of experimental conditions. Thus, it is very

Table 4-15. Biodegradation Rate Constants/Half-Lives for Benzene

Half-life (day)	Rate Constant ^(a) (day ⁻¹)	Reported Value	Reported Units	Reported Uncertainty	Experimental Medium	Technique (Conditions)	Reference	Source Cited
16	0.44	0.44	day ⁻¹	NR	Surface (river) water	Measured; (aerobic) ^(b)	U.S. PHS, 1991	Vaishnav and Babeu, 1987
8	0.082	0.082	day ⁻¹	NR	Surface (harbor) water	Measured; (aerobic) ^(c) + enrichment	U.S. PHS, 1991	Vaishnav and Babeu, 1987
		no degradation			Surface (harbor) water	Measured; (aerobic) ^(d)	U.S. PHS, 1991	Vaishnav and Babeu, 1987
28	0.025	0.025	day ⁻¹	NR	Groundwater	Measured; (aerobic) ^(e)	U.S. PHS, 1991	Vaishnav and Babeu, 1987
73 ^(b)	0.0095	0.0095	day ⁻¹	NR	Groundwater (field) ^(f)	Measured; (aerobic) ^(g)	U.S. PHS, 1991	Chiang et al., 1989
2 ^(b)	0.317 ^(b)				Groundwater (lab)	Measured; (aerobic) ^(h) + enrichment	U.S. PHS, 1991	Karlson and Frankenberger, 1989
0.7 ^(b)	0.956 ^(b)				Groundwater (lab)	Measured; (aerobic) + enrichment	U.S. PHS, 1991	Karlson and Frankenberger, 1989
		complete degradation		NR	Aquifer material	Measured; (aerobic) + nitrate	U.S. PHS, 1991	Major et al., 1988
10 ^(b)	0.07 ^(m)			NR	Aquifer material	Measured; (aerobic)	U.S. PHS, 1991	Major et al., 1988
6 ^(b)	0.11	0.11	day ⁻¹	NR	Aquatic systems	NR	Lyman, 1990; Hatterer-Frey and Travis, 1990	Lee and Ryan, 1979

Table 4-15. Biodegradation Rate Constants/Half-Lives for Benzene
(Continued)

Half-life (day)	Rate Constant ^(a) (day ⁻¹)	Reported Value	Reported Units	Reported Uncertainty	Experimental Medium	Technique (Conditions)	Reference	Source Cited
154 ^(b)	0.0045 ^(b)			NR	Aquifer material	Measured; (anaerobic) ^(b)	U.S. PHS, 1991	Wilson et al., 1986
462 ^(b)	0.0015 ^(b)			NR	Aquifer material	Measured; (anaerobic) ^(b)	U.S. PHS, 1991	Wilson et al., 1986
231 ^(b)	0.003 ^(b)			NR	Aquifer material	Measured; (anaerobic)	U.S. PHS, 1991	Major et al., 1988
16 ^(b)	0.044 ^(b)			NR	Aquifer material	Measured; (anaerobic) + nitrate	U.S. PHS, 1991	Major et al., 1988
17 ^(b)	0.04	0.04	day ⁻¹	NR	Seawater	Calculated ^(c) ; (aerobic)	Wakeham et al., 1986	Wakeham et al., 1986
0.4 ^(b)	1.67	1.67	day ⁻¹	NR	Seawater	Calculated ^(c) ; (aerobic)	Wakeham et al., 1986	Wakeham et al., 1986
0.4 ^(b)	1.66	1.66	day ⁻¹	NR	Seawater	Measured; (aerobic)	Wakeham et al., 1986	Wakeham et al., 1986
7 ^(b)	0.096 ^(b)			NR	Domestic wastewater	Measured; (aerobic) + enrichment	U.S. PHS, 1991	Tabak et al., 1981
0.07 ^(b)	10.1 ^(b)			NR	Industrial wastewater	Measured; (aerobic) + enrichment	U.S. PHS, 1991	Davis et al., 1981
103 ^(b)	0.0067	278 × 10 ⁻⁴	hr ⁻¹	NR	Soil/sediment	NR	Hattemer-Frey and Travis, 1990	Tucker et al., 1986

Table 4-15. Biodegradation Rate Constants/Half-Lives for Benzene
(Continued)

Half-life (day)	Rate Constant ^(a) (day ⁻¹)	Reported Value	Reported Units	Reported Uncertainty	Experimental Medium	Technique (Conditions)	Reference	Source Cited
26 ^(b)	0.026 ^(c)			NR	Soil	Measured; (aerobic)	U.S. PHS, 1991	Haider et al., 1981
18 ^(b)	0.039 ^(c)	NA	NA	NR	Soil	Measured; (aerobic)	U.S. PHS, 1991	Haider et al., 1981
21 ^(b)	0.033 ^(c)	NA	NA	NR	Soil	Measured; (aerobic)	U.S. PHS, 1991	Haider et al., 1981
43 ^(b)	0.016 ^(c)	NA	NA	NR	Soil	Measured; (aerobic)	U.S. PHS, 1991	Haider et al., 1981
77 ^(b)	0.009 ^(c)	NA	NA	NR	Soil	Measured; (aerobic)	U.S. PHS, 1991	Haider et al., 1991

NR = Not Reported.

(a) If the value for the rate constant was not reported, it was calculated, whenever it was feasible, based on given information in the research paper using the equation

$$\ln \frac{C}{C_0} = -kt \quad \text{where } C_0 = \text{initial benzene concentration (t = 0), } C = \text{benzene concentration at the time t, } k = \text{rate constant, } t = \text{time period.}$$

- (b) No supplements added; pH = 7.76.
- (c) Enriched with nutrients and acclimated microbes; pH = 7.56.
- (d) No supplements added; pH = 7.56.
- (e) No supplements added; pH = 8.23.
- (f) Sampling groundwater in shallow aquifer at monitoring wells.
- (g) From material balance and non-linear least-squares analyses of field results from 3-year sampling period.
- (h) Half-life ($t_{1/2}$) was calculated using Eq. $t_{1/2} = \ln 2/k$; k = rate constant.

Table 4-15. Biodegradation Rate Constants/Half-Lives for Benzene
(Continued)

(i)	Gasoline-contaminated groundwater + N source added; pH = 7.93, T = 296K.
(j)	<p>Degradation rate:</p> $\left(\frac{dc}{dt}\right) = 12.7 \mu\text{g L}^{-1} \text{h}^{-1}$ <p>control: $6.4 \mu\text{g L}^{-1} \text{h}^{-1}$</p> $\left(\frac{dc}{dt}\right) = -kC_o$ $C_o = 477 \mu\text{g/L}$ $k = \left(\frac{12.7 - 6.4}{477}\right) \times 24 [\text{day}^{-1}]$
(k)	Gasoline-contaminated groundwater + N source + enriched culture of hydrocarbon oxidizer; pH = 7.93, T = 296K.
(l)	<p>Degradation rate:</p> $\left(\frac{dc}{dt}\right) = 25.4 \mu\text{g L}^{-1} \text{h}^{-1}$ <p>control: $6.4 \mu\text{g L}^{-1} \text{h}^{-1}$</p> $\frac{dc}{dt} = -kC_o$ $C_o = 477 \mu\text{g/L}$ $k = \left(\frac{25.4 - 6.4}{477}\right) \times 24 [\text{day}^{-1}]$
(m)	$C_o = 79\%$; $C = 1\%$; $t = 62$ days; $\ln \frac{1}{79} = -k \times 62$
(n)	T = 290K; pH = 7.3.

Table 4-15. Biodegradation Rate Constants/Half-Lives for Benzene
(Continued)

(o)	$C_o = 100\%$; $C = 28\%$; $t \approx 40$ weeks; $\ln \frac{28}{100} = -k \times 40 \times 7$
(p)	$C_o = 100\%$; $C = 1\%$; $t = 120$ weeks; $\ln \frac{1}{100} = -k \times 120 \times 7$
(q)	$C_o = 79\%$; $C = 66\%$; $t = 62$ days; $\ln \frac{66}{79} = -k \times 62$
(r)	$C_o = 79\%$; $C = 5\%$; $t = 62$ days; $\ln \frac{5}{79} = -k \times 62$
(s)	$k_b = k_{\text{obs}}(\text{VOC}) - k_r(\text{VOC})$ $k_{(\text{VOC})} = f k_{\text{ref}(12)} (D_{\text{VOC}})^{1/2} (D_{\text{F}12})^{1/2}$
(t)	$C_o = 100\%$; $C = 51\%$; $t = 7$ days; $\ln \frac{51}{100} = -k \times 7$
(u)	$C_o = 50$ mg/L; $C = 4$ mg/L; $t = 6$ h; $\ln \frac{4}{50} = -k \times \frac{6}{24}$
(v)	$C_o = 100\%$; $C = 92.5\%$; $t = 3$ days; $\ln \frac{92.5}{100} = -k \times 3$
(w)	$C_o = 100\%$; $C = 76\%$; $t = 7$ days; $\ln \frac{76}{100} = -k \times 7$
(x)	$C_o = 100\%$; $C = 63\%$; $t = 14$ days; $\ln \frac{63}{100} = -k \times 14$
(y)	$C_o = 100\%$; $C = 56\%$; $t = 35$ days; $\ln \frac{56}{100} = -k \times 35$
(z)	$C_o = 100\%$; $C = 53\%$; $t = 70$ days; $\ln \frac{53}{100} = -k \times 70$

difficult to derive a single value for the biodegradation rate constant and the corresponding half-life for benzene.

5.0 CONCLUSIONS AND RECOMMENDATIONS

A summary of representative values of intermedia transfer factors and estimation method is given in Table 1-1. This section discusses areas in which the estimation and use of intermedia transfer parameters could be refined to increase the accuracy of multipathway exposure assessment.

Physicochemical Parameters

Among the physicochemical parameters recommended in this report for multimedia analysis of benzene (i.e., solubility, vapor pressure, molar volume, boiling point, and molecular weight), the experimentally derived aqueous solubility is particularly important because it can be used to predict chemical-specific K_{oc} , K_{ow} , and BCF values. Although solubility is site specific (i.e., it depends on pH, temperature, and pressure), under common environmental conditions, the site-specific variability of the aqueous solubility may be needed to be considered. Nonetheless, knowledge of solubility as a function of temperature will allow the estimate of K_{ow} at different temperatures (from K_{ow} solubility correlations) when the temperature dependence of K_{ow} is unknown.

Partition Coefficients

Experimentally determined partition coefficients for benzene are presented in this report for Henry's Law constant, K_{ow} , K_{oc} , BCFs for various aquatic organisms, and root uptake. However, measured values for the air-to-leaf partition coefficient and other biotransfer factors which address partitioning through food uptake were not found in the literature. Based on the current study, it is believed that the partitioning of benzene to vegetation via the air-to-leaf mechanism of airborne benzene (presently not included in the CAPCOA model) may be a significant pathway for accumulation of airborne benzene in leafy vegetation. Although various prediction equations to calculate partition coefficients have been found in the literature, values are presented only for those correlations

considered applicable to benzene or homologous compounds (except where noted). The use of the full range of partition coefficients and prediction equations presented in this report may be used to augment the approach used by the CAPCOA (1992) guidelines.

Biotransfer Factors

The concept of B_{TFs} for milk, beef, eggs, and vegetables should be revisited since it is based implicitly on the assumption of steady state conditions. For instance, the popular biotransfer correlations proposed by Travis and Arms (1988) were derived by pooling data from a number of independent studies. Thus, the original data could be reanalyzed to determine the degree to which the independent studies were performed at comparable feed concentrations, time intervals, and animal ages and activity, since these and other experimental variables can influence the point at which steady state may be reached. In addition, the original studies from which Travis and Arms (1988) derived their correlations for B_{TFs} did not include benzene as a study compound, and did not consider inhalation as a pathway for bioaccumulation in meat, and milk.

Intermedia Transport Parameters

Although a measured value for the dry deposition velocity of benzene was not found in the literature, it can be estimated as discussed in Section 4.3.3. Sehmel (1980) and Davidson and Wu (1989) critically reviewed experimentally measured deposition velocities for other gaseous compounds (such as criteria air pollutants) and reported variability of the dry deposition velocity over two orders of magnitude, depending on the deposition surface and other factors. Thus, estimates of the dry deposition velocity should consider the appropriate meteorological conditions and surface type.

Degradation

While biodegradation is the most important transformation process in most types of soil, the biodegradation process depends on numerous different factors that it may be

inappropriate to characterize the biodegradation half-life of benzene by a single default value (see Section 4.4.2).

Finally, it is worth noting that the major degradation process for benzene is in the atmosphere by reaction with hydroxyl radicals. The reaction half-life for this process is estimated at 6.5 days. Therefore, when the atmospheric concentration of benzene is determined using atmospheric dispersion models, it is important to consider the atmospheric degradation of benzene when the relevant convective residence times are of the order of a day or more.

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